## NCIPLOT: A Program for Plotting Noncovalent Interact

Journal of Chemical Theory and Computation 7, 625-632 DOI: 10.1021/ct100641a

Citation Report

#	Article	IF	CITATIONS
39	On the dimerization of chlorophyll in photosystem II. Physical Chemistry Chemical Physics, 2011, 13, 16022.	1.3	17
40	A Hirshfeld Partitioning of the MP2 Correlation Energy: Method and Its Application to the Benzene Dimers. Journal of Chemical Theory and Computation, 2011, 7, 2049-2058.	2.3	4
41	Chiral Sulfinamide/Achiral Sulfonic Acid Cocatalyzed Enantioselective Protonation of Enol Silanes. Organic Letters, 2011, 13, 4260-4263.	2.4	46
42	Analysis of Hydrogen-Bond Interaction Potentials from the Electron Density: Integration of Noncovalent Interaction Regions. Journal of Physical Chemistry A, 2011, 115, 12983-12990.	1.1	339
43	A Potent Ruthenium(II) Antitumor Complex Bearing a Lipophilic Levonorgestrel Group. Inorganic Chemistry, 2011, 50, 9164-9171.	1.9	74
44	Intramolecular OHâ⊄Ï€ interactions in alkenols and alkynols. Physical Chemistry Chemical Physics, 2011, 13, 14183.	1.3	47
45	A novel method for quantitatively predicting non-covalent interactions from protein and nucleic acid sequence. Journal of Molecular Graphics and Modelling, 2011, 31, 28-34.	1.3	6
46	Revealing non-covalent interactions in solids: NCI plots revisited. Physical Chemistry Chemical Physics, 2012, 14, 12165.	1.3	279
47	Adsorption of Organic Molecules on Kaolinite from the Exchange-Hole Dipole Moment Dispersion Model. Journal of Chemical Theory and Computation, 2012, 8, 5124-5131.	2.3	50
48	Aminoindolines versus Quinolines: Mechanistic Insights into the Reaction between 2-Aminobenzaldehydes and Terminal Alkynes in the Presence of Metals and Secondary Amines. Journal of Organic Chemistry, 2012, 77, 6179-6185.	1.7	22
49	Photochemistry of Tetrasulfur Tetranitride: Laser Flash Photolysis and Quantum Chemical Study. Inorganic Chemistry, 2012, 51, 4747-4755.	1.9	6
50	Catalytic Mechanism of 4-Oxalocrotonate Tautomerase: Significances of Protein–Protein Interactions on Proton Transfer Pathways. Journal of Physical Chemistry B, 2012, 116, 6889-6897.	1.2	7
51	Density-Functional Errors in Alkanes: A Real-Space Perspective. Journal of Chemical Theory and Computation, 2012, 8, 2676-2681.	2.3	16
52	Coupling Quantum Interpretative Techniques: Another Look at Chemical Mechanisms in Organic Reactions. Journal of Chemical Theory and Computation, 2012, 8, 3993-3997.	2.3	104
53	A computational study of the enantioselective addition of n-BuLi to benzaldehyde in the presence of a chiral lithium N,P amide. Organic and Biomolecular Chemistry, 2012, 10, 2807.	1.5	12
54	<i>In Silico</i> Modeling of the Molecular Structure and Binding of Leukotriene A4 into Leukotriene A4 Hydrolase. Chemical Biology and Drug Design, 2012, 80, 902-908.	1.5	3
55	Highly selective mercury(ii) cations detection in mixed–aqueous media by a ferrocene-based fluorescent receptor. Dalton Transactions, 2012, 41, 4437.	1.6	27
56	The Nature of Transannular Interactions in E4N4 and E82+ (E = S, Se). Journal of Chemical Theory and Computation, 2012, 8, 4249-4258.	2.3	13

#	Article	IF	CITATIONS
57	Tuning Nonlinear Optical and Optoelectronic Properties of Vinyl Coupled Triazene Chromophores: A Density Functional Theory and Time-Dependent Density Functional Theory Investigation. Journal of Physical Chemistry A, 2012, 116, 4667-4677.	1.1	164
58	lonic interactions: Comparative topological approach. Computational and Theoretical Chemistry, 2012, 998, 193-201.	1.1	41
59	Adsorption of <scp>l</scp> -DOPA Intercalated in Hydrated Na-Saponite Clay: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2012, 116, 26414-26421.	1.5	25
60	Density-decomposed orbital-free density functional theory for covalently bonded molecules and materials. Physical Review B, 2012, 86, .	1.1	42
61	Modulating the Strength of Hydrogen Bonds through Beryllium Bonds. Journal of Chemical Theory and Computation, 2012, 8, 2293-2300.	2.3	81
62	Computational Prediction of Residues Involved in Fidelity Checking for DNA Synthesis in DNA Polymerase I. Biochemistry, 2012, 51, 2569-2578.	1.2	29
63	Estimating stacking interaction energy using atom in molecules properties: Homodimers of benzene and pyridine. International Journal of Quantum Chemistry, 2012, 112, 3008-3017.	1.0	10
64	The reduced density gradient in atoms. International Journal of Quantum Chemistry, 2012, 112, 3594-3598.	1.0	27
65	Molecular Balances Based on Aliphatic CHâ^'Ï€ and Lone-Pairâ^'Ï€ Interactions. Journal of Physical Chemistry Letters, 2012, 3, 1493-1496.	2.1	78
66	Toward a ligand specific of Pb2+ with respect to the Zn2+ and Ca2+ cations: A track from quantum chemistry. Chemical Physics Letters, 2012, 532, 9-12.	1.2	2
67	<i>t</i> Bu or not <i>t</i> Bu?. Chemistry - A European Journal, 2012, 18, 1640-1649.	1.7	35
68	Multiwfn: A multifunctional wavefunction analyzer. Journal of Computational Chemistry, 2012, 33, 580-592.	1.5	21,818
69	H-H interaction in phenanthrene: Attraction or repulsion?. Journal of Structural Chemistry, 2013, 54, 479-483.	0.3	19
70	Describing curved–planar π–π interactions: modeled by corannulene, pyrene and coronene. Physical Chemistry Chemical Physics, 2013, 15, 12694.	1.3	37
71	On the Importance of Anion–π Interactions in the Mechanism of Sulfide:Quinone Oxidoreductase. Chemistry - an Asian Journal, 2013, 8, 2708-2713.	1.7	31
72	QM/MM description of platinum–DNA interactions: comparison of binding and DNA distortion of five drugs. RSC Advances, 2013, 3, 4066.	1.7	30
73	Impact of functionalized linkers on the energy landscape of ZIFs. CrystEngComm, 2013, 15, 9603.	1.3	28
74	Intramolecular Interactions in 2-Aminoethanol and 3-Aminopropanol. Journal of Physical Chemistry A, 2013, 117, 10260-10273.	1.1	40

#	Article	IF	CITATIONS
75	Modulating weak intramolecular interactions through the formation of beryllium bonds: complexes between squaric acid and BeH2. Journal of Molecular Modeling, 2013, 19, 2759-2766.	0.8	24
76	Hemichelation, a Way To Stabilize Electron-Unsaturated Complexes: The Case of T-Shaped Pd and Pt Metallacycles Journal of the American Chemical Society, 2013, 135, 17839-17852.	6.6	28
77	Features of three-centered hydrogen bonding in di(vinylpyrrolyl)pyridine and di(vinylpyridyl)-pyrrole from the ab initio calculation data and QTAIM analysis. Journal of Structural Chemistry, 2013, 54, 651-659.	0.3	2
78	On the Nature of Hypercoordination in Dihalogenated Perhalocyclohexasilanes. Journal of Physical Chemistry A, 2013, 117, 3529-3538.	1.1	27
79	Large negative thermal expansion of a polymer driven by a submolecular conformational change. Nature Chemistry, 2013, 5, 1035-1041.	6.6	103
80	Easy methods to study the smart energetic TNT/CL-20 co-crystal. Journal of Molecular Modeling, 2013, 19, 4909-4917.	0.8	67
81	Enhancing Effects of Electron-Withdrawing Groups and Metallic Ions on Halogen Bonding in the YC <sub>6</sub> F <sub>4</sub> X···C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> (X = Cl, Br, I; Y = F, CN,) 2013, 117, 12959-12968.	Tj FTQq0 (	) 0.rgBT /Ove
82	Structure-directed functional properties of symmetrical and unsymmetrical Br-substituted Schiff-bases. Journal of Molecular Structure, 2013, 1049, 377-385.	1.8	15
83	Intramolecular hydrogen bond C-Hâ<¯N in 1,1′-divinyl-2,2′-diimidazolyl according to the data of ab initio calculations and QTAIM analysis. Journal of Structural Chemistry, 2013, 54, 1029-1033.	0.3	4
84	Influence of 2′-Fluoro versus 2′- <i>O</i> -Methyl Substituent on the Sugar Puckering of 4′- <i>C</i> -Aminomethyluridine. Journal of Organic Chemistry, 2013, 78, 9956-9962.	1.7	23
85	Coordination of CO to low-valent phosphorus centres and other related P–C bonding situations. A theoretical case study. Chemical Science, 2013, 4, 4309.	3.7	27
86	Bis(carbazolyl)ureas as Selective Receptors for the Recognition of Hydrogenpyrophosphate in Aqueous Media. Journal of Organic Chemistry, 2013, 78, 9725-9737.	1.7	29
87	C–Hâ<Ï€ interactions as modulators of carbocation structure – implications for terpene biosynthesis. Chemical Science, 2013, 4, 2512.	3.7	45
88	<i>NCImilano</i> : an electron-density-based code for the study of noncovalent interactions. Journal of Applied Crystallography, 2013, 46, 1513-1517.	1.9	50
89	Computational insights on the mechanism of the catalytic hydrogenation with BINAP–diamine–Ru complexes: the role of base and origin of selectivity. Chemical Communications, 2013, 49, 4277-4279.	2.2	16
90	Halogen Bonding from a Hard and Soft Acids and Bases Perspective: Investigation by Using Density Functional Theory Reactivity Indices. Chemistry - A European Journal, 2013, 19, 519-530.	1.7	109
91	Synthesis and Structural Characterization of Various N,O,N-Chelated Aluminum and Gallium Complexes for the Efficient ROP of Cyclic Esters and Carbonates: How Do Aluminum and Gallium Derivatives Compare ?. Organometallics, 2013, 32, 587-598.	1.1	91
92	Topology Switching in [32]Heptaphyrins Controlled by Solvent, Protonation, and <i>meso</i> â€Substituents. Chemistry - A European Journal, 2013, 19, 1617-1628.	1.7	49

#	Article	IF	CITATIONS
93	Theoretical investigation on the electronic and optical properties of diarylfluorene-based π-stacked molecules as supramolecular semiconductors. Chemical Physics Letters, 2013, 578, 150-155.	1.2	4
94	Benzophenone and DNA: Evidence for a Double Insertion Mode and Its Spectral Signature. Journal of Physical Chemistry Letters, 2013, 4, 4119-4124.	2.1	42
95	Weak intramolecular OHâ∢Ï€ hydrogen bonding in methallyl- and allyl-carbinol. Chemical Physics Letters, 2013, 582, 31-37.	1.2	13
96	On critical points and exchange-related properties of intramolecular bonds between two electronegative atoms. Chemical Physics Letters, 2013, 579, 122-126.	1.2	31
97	<b>Molecular Switching Behavior in Isosteric DNA Base Pairs</b> . ChemPhysChem, 2013, 14, 1219-1226.	1.0	12
98	Efficient and Accurate Theoretical Methods To Investigate Anion-Ï€ Interactions in Protein Model Structures. Journal of Physical Chemistry B, 2013, 117, 3315-3322.	1.2	26
99	What Stabilizes the Li <sub><i>n</i></sub> P <sub><i>n</i></sub> Inorganic Double Helices?. Journal of Physical Chemistry Letters, 2013, 4, 1018-1022.	2.1	30
100	Noncovalent Interaction Analysis in Fluctuating Environments. Journal of Chemical Theory and Computation, 2013, 9, 2226-2234.	2.3	150
101	Halogen Bonds: Benchmarks and Theoretical Analysis. Journal of Chemical Theory and Computation, 2013, 9, 1918-1931.	2.3	435
102	An Interplay of Cooperativity between Cationâ‹â‹ï€, Anionâ‹â‹â‹ï€ and CHâ‹â‹â‹Anion Intera 2013, 14, 1149-1154.	ctions. Ch 1.0	emPhysChen 14
103	Toward a Deeper Understanding of Enzyme Reactions Using the Coupled ELF/NCI Analysis: Application to DNA Repair Enzymes. Journal of Chemical Theory and Computation, 2013, 9, 2156-2160.	2.3	48
104	Could an anisotropic molecular mechanics/dynamics potential account for sigma hole effects in the complexes of halogenated compounds?. Journal of Computational Chemistry, 2013, 34, 1125-1135.	1.5	21
105	Conformational Control in [22]- and [24]Pentaphyrins(1.1.1.1.1) by Meso Substituents and their N-Fusion Reaction. Journal of Organic Chemistry, 2013, 78, 4419-4431.	1.7	25
106	Mechanism and Selectivity of Bioinspired Cinchona Alkaloid Derivatives Catalyzed Asymmetric Olefin Isomerization: A Computational Study. Journal of the American Chemical Society, 2013, 135, 7462-7473.	6.6	69
107	<i>Ab Initio</i> QM/MM Calculations Show an Intersystem Crossing in the Hydrogen Abstraction Step in Dealkylation Catalyzed by AlkB. Journal of Physical Chemistry B, 2013, 117, 6410-6420.	1.2	58
108	Intramolecular halogen–halogen bonds?. Physical Chemistry Chemical Physics, 2013, 15, 11543.	1.3	61
109	Revealing noncovalent interactions in quantum crystallography: Taurine revisited. Journal of Computational Chemistry, 2013, 34, 466-470.	1.5	17
110	A new theoretical analysis of the cooperative effect in T-shaped hydrogen complexes of CnHmâ^™â^™â^™HCNâ^ with n = 2, m = 2 or 4, and W = F or CN. Journal of Molecular Modeling, 2013, 19, 35.	™â^™â^™  51-35 <u>68.</u>	HW

0						
	ΓΑΤ	ION	R	EΡ	0	RT

#	Article	IF	CITATIONS
111	Controlling Conformations of Conjugated Polymers and Small Molecules: The Role of Nonbonding Interactions. Journal of the American Chemical Society, 2013, 135, 10475-10483.	6.6	386
112	Experimental and theoretical studies on the coordination chemistry of the N1-hexyl substituted pyrimidines (uracil, 5-fluorouracil and cytosine). Dalton Transactions, 2013, 42, 7631.	1.6	12
113	Conformational preferences of RCH2CH2CN (RÂ=ÂCH3, F, Cl) cyanides and their corresponding isocyanides. Structural Chemistry, 2013, 24, 1789-1798.	1.0	3
114	New Insights on the Molecular Recognition of Imidacloprid with Aplysia californica AChBP: A Computational Study. Journal of Physical Chemistry B, 2013, 117, 3944-3953.	1.2	20
115	Extreme density-driven delocalization error for a model solvated-electron system. Journal of Chemical Physics, 2013, 139, 184116.	1.2	93
116	Prediction of protein-peptide interactions: application of the XPairIt API to anthrax lethal factor and substrates. Proceedings of SPIE, 2013, , .	0.8	0
117	Novel Alkoxide Cluster Topologies Featuring Rare Seesaw Geometry at Transition Metal Centers. Chemistry - A European Journal, 2013, 19, 12225-12228.	1.7	31
118	Conformational analysis of 2,2-difluoroethylamine hydrochloride: double <i>gauche</i> effect. Beilstein Journal of Organic Chemistry, 2014, 10, 877-882.	1.3	9
119	Deformation density components analysis of fullerene-based anti-HIV drugs. Journal of Molecular Modeling, 2014, 20, 2486.	0.8	3
120	Host–Guest Interactions in ExBox <sup>4+</sup> . ChemPhysChem, 2014, 15, 4108-4116.	1.0	19
121	Interplay between non-covalent interactions in complexes and crystals with halogen bonds. Russian Chemical Reviews, 2014, 83, 1181-1203.	2.5	168
122	Relationships between Th1 or Th2 iNKT Cell Activity and Structures of CD1d-Antigen Complexes: Meta-analysis of CD1d-Glycolipids Dynamics Simulations. PLoS Computational Biology, 2014, 10, e1003902.	1.5	5
123	Multifunctional Benzothiadiazoleâ€Based Small Molecules Displaying Solvatochromism and Sensing Properties toward Nitroarenes, Anions, and Cations. ChemistryOpen, 2014, 3, 242-249.	0.9	21
124	First Stabilization of 14â€Electron Rhodium(I) Complexes by Hemichelation. Angewandte Chemie - International Edition, 2014, 53, 9827-9831.	7.2	23
125	Similar Strength of the NH···O and NH···S Hydrogen Bonds in Binary Complexes. Journal of Physical Chemistry A, 2014, 118, 11074-11082.	1.1	57
126	Reactivity of low-oxidation state tin compounds: an overview of the benefits of combining DFT Theory and experimental NMR spectroscopy. Canadian Journal of Chemistry, 2014, 92, 447-461.	0.6	1
127	Spatial assignment of symmetry adapted perturbation theory interaction energy components: The atomic SAPT partition. Journal of Chemical Physics, 2014, 141, 044115.	1.2	76
128	JANPA: An open source cross-platform implementation of the Natural Population Analysis on the Java platform. Computational and Theoretical Chemistry, 2014, 1050, 15-22.	1.1	108

#	Article	IF	CITATIONS
129	3-Picoline Mediated Self-Assembly of M(II)–Malonate Complexes (M = Ni/Co/Mn/Mg/Zn/Cu) Assisted by Various Weak Forces Involving Lone Pairâ'ï€, ï€â€"ï€, and Anion··΀–Hole Interactions. Journal of Physical Chemistry B, 2014, 118, 14713-14726.	1.2	81
130	Catalytic Enantioselective Alkylation of Sulfenate Anions to Chiral Heterocyclic Sulfoxides Using Halogenated Pentanidium Salts. Angewandte Chemie - International Edition, 2014, 53, 11849-11853.	7.2	138
131	Stereoselectivity through a network of non-classical CH weak interactions: a prospective study of a bicyclic organocatalytic scaffold. New Journal of Chemistry, 2014, 38, 5975-5982.	1.4	5
132	Polarizable molecular mechanics studies of <scp>Cu(I)/Zn(II)</scp> superoxide dismutase: Bimetallic binding site and structured waters. Journal of Computational Chemistry, 2014, 35, 2096-2106.	1.5	9
133	Significant evidence of C⋯O and C⋯C long-range contacts in several heterodimeric complexes of CO with CH <sub>3</sub> –X, should one refer to them as carbon and dicarbon bonds!. Physical Chemistry Chemical Physics, 2014, 16, 17238-17252.	1.3	56
134	Charge density analysis for crystal engineering. Chemistry Central Journal, 2014, 8, 68.	2.6	42
135	Computational Study of Putative Residues Involved in DNA Synthesis Fidelity Checking in Thermus aquaticus DNA Polymerase I. Advances in Protein Chemistry and Structural Biology, 2014, 96, 39-75.	1.0	12
136	Progressive compression of 1,ï‰-diammonium-alkanes inside a rigid crystalline molecular cage. Chemical Communications, 2014, 50, 14086-14088.	2.2	19
137	Substituent effects in cation–π interactions revisited: a general approach based on intrinsic properties of the arenes. Physical Chemistry Chemical Physics, 2014, 16, 1322-1326.	1.3	28
138	Dimers of Nâ€Heterocyclic Carbene Copper, Silver, and Gold Halides: Probing Metallophilic Interactions through Electron Density Based Concepts. Chemistry - A European Journal, 2014, 20, 734-744.	1.7	42
139	Critic2: A program for real-space analysis of quantum chemical interactions in solids. Computer Physics Communications, 2014, 185, 1007-1018.	3.0	497
140	αâ€Halogenoacetanilides as Hydrogenâ€Bonding Organocatalysts that Activate Carbonyl Bonds: Fluorine versus Chlorine and Bromine. Chemistry - A European Journal, 2014, 20, 2849-2859.	1.7	17
141	Understanding the Fundamental Role of ï€ <i>/</i> ï€, ïƒ <i>/</i> ïƒ, and ïƒ <i>/</i> ï€ Dispersion Interactions in Shaping Carbonâ€Based Materials. Chemistry - A European Journal, 2014, 20, 4931-4941.	1.7	109
142	Experimental and Theoretical Studies of Intramolecular Hydrogen Bonding in 3-Hydroxytetrahydropyran: Beyond AIM Analysis. Journal of Physical Chemistry A, 2014, 118, 2794-2800.	1.1	18
143	Mukaiyama–Michael Reactions with <i>trans</i> â€2,5â€Diarylpyrrolidine Catalysts: Enantioselectivity Arises from Attractive Noncovalent Interactions, Not from Steric Hindrance. Chemistry - A European Journal, 2014, 20, 5983-5993.	1.7	48
144	A Novel N,P,C Cage Complex Formed by Rearrangement of a Tricyclic Phosphirane Complex: On the Importance of Nonâ€covalent Interactions. Chemistry - A European Journal, 2014, 20, 7010-7016.	1.7	19
145	Solid‣tate Hierarchical Cyclodextrinâ€Based Supramolecular Polymer Constructed by Primary, Secondary, and Tertiary Azido Interactions. Angewandte Chemie - International Edition, 2014, 53, 7238-7242.	7.2	19
146	Anionâ‹â‹â‹Si Interactions in an Inverse Sandwich Complex: A Computational Study. ChemPhysChem, 2014, 912-917.	15 1.0	12

~		<u> </u>	
$(   \mathbf{T} \wedge \mathbf{T} \rangle$	γιον Ι	VEDO	דסר
CITA		NLPV	ואכ

#	Article	IF	CITATIONS
147	Polar and stereoelectronic effects on the structural and spectroscopic properties of halomethanols. Computational and Theoretical Chemistry, 2014, 1037, 49-52.	1.1	6
148	Exploring non-covalent interactions in guanine- and xanthine-based model DNA quadruplex structures: a comprehensive quantum chemical approach. Physical Chemistry Chemical Physics, 2014, 16, 2072-2084.	1.3	62
149	Computational study of diastereoselective ortho-lithiations of chiral ferrocenes. Organic and Biomolecular Chemistry, 2014, 12, 132-140.	1.5	12
150	Following the Molecular Mechanism for the NH <sub>3</sub> + LiH â†' LiNH <sub>2</sub> + H <sub>2</sub> Chemical Reaction: A Study Based on the Joint Use of the Quantum Theory of Atoms in Molecules (QTAIM) and Noncovalent Interaction (NCI) Index. Journal of Physical Chemistry A, 2014, 118, 1663-1672.	1.1	61
151	Gauche Preference of β-Fluoroalkyl Ammonium Salts. Journal of Physical Chemistry A, 2014, 118, 503-507.	1.1	15
152	Unraveling non-covalent interactions within flexible biomolecules: from electron density topology to gas phase spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 9876.	1.3	156
153	AlgoGen: A tool coupling a linear-scaling quantum method with a genetic algorithm for exploring non-covalent interactions. Computational and Theoretical Chemistry, 2014, 1028, 7-18.	1.1	15
154	Novel non-covalent interactions involved with the Al <sub>13</sub> M cluster (M = Li, Na, K, Cu, Ag,) Tj ETQq1 1	0.784314 0.8	rg&T /Overlo
155	Trends in Physisorption of Ionic Liquids on Boron-Nitride Sheets. Journal of Physical Chemistry C, 2014, 118, 26003-26016.	1.5	54
156	Regioselectivity of Intermolecular Pauson–Khand Reaction of Aliphatic Alkynes: Experimental and Theoretical Study of the Effect of Alkyne Polarization. Journal of Organic Chemistry, 2014, 79, 10999-11010.	1.7	21
157	Comparative estimation of the energies of intramolecular C-H…O, N-H…O, and O-H…O hydrogen bonds according to the QTAIM analysis and NMR spectroscopy data. Journal of Structural Chemistry, 2014, 55, 636-643.	0.3	19
158	Heavy Element Metallacycles: Insights into the Nature of Host–Guest Interactions Involving Dihalide Mercuramacrocycle Complexes. Journal of Physical Chemistry C, 2014, 118, 28244-28251.	1.5	20
159	Alternative Pathway for the Reaction Catalyzed by DNA Dealkylase AlkB from Ab Initio QM/MM Calculations. Journal of Chemical Theory and Computation, 2014, 10, 5136-5148.	2.3	32
160	Interaction of Polycationic Ni(II)-Salophen Complexes with G-Quadruplex DNA. Inorganic Chemistry, 2014, 53, 12519-12531.	1.9	44
161	A combined experimental and computational study of supramolecular assemblies in ternary copper( <scp>ii</scp> ) complexes with a tetradentate N <sub>4</sub> donor Schiff base and halides. RSC Advances, 2014, 4, 58643-58651.	1.7	29
162	Density-functional description of electrides. Physical Chemistry Chemical Physics, 2014, 16, 14584-14593.	1.3	76
163	The Houk–List transition states for organocatalytic mechanisms revisited. Chemical Science, 2014, 5, 2057-2071.	3.7	154
164	Nucleic Acid Quadruplexes Based on 8-Halo-9-deazaxanthines: Energetics and Noncovalent Interactions in Quadruplex Stems. Journal of Chemical Theory and Computation, 2014, 10, 5353-5365.	2.3	19

#	Article	IF	CITATIONS
165	Mechanistic understanding of domino cyclization between gem-dialkylthio vinylallenes and benzylamine towards economic synthesis: a computational study. Green Chemistry, 2014, 16, 2653.	4.6	27
166	Theoretical analysis of the intermolecular interactions in naphthalene diimide and pyrene complexes. Physical Chemistry Chemical Physics, 2014, 16, 24216-24222.	1.3	36
167	Direct observation of a lithiated oxirane: a synergistic study using spectroscopic, crystallographic, and theoretical methods on the structure and stereodynamics of lithiated ortho-trifluoromethyl styrene oxide. Chemical Science, 2014, 5, 528-538.	3.7	50
168	The nature of hydrogen bonding in <i>R</i> <sup>2</sup> <sub>2</sub> (8) crystal motifs – a computational exploration. Molecular Physics, 2014, 112, 3195-3205.	0.8	14
170	Investigation of putative arene-C–Hâ<ï€(quasi-chelate ring) interactions in copper( <scp>i</scp> ) crystal structures. Chemical Communications, 2014, 50, 5984-5986.	2.2	42
171	Design of coordination polymers with 4â€2-substituted functionalized terpyridyls in the backbone and pendent cyclopentadienyliron moieties. Polymer Chemistry, 2014, 5, 3453-3465.	1.9	23
172	Revisiting H <sub>2</sub> O Nucleation around Au <sup>+</sup> and Hg <sup>2+</sup> : The Peculiar "Pseudo-Soft―Character of the Gold Cation. Journal of Chemical Theory and Computation, 2014, 10, 1900-1909.	2.3	7
173	An anatomy of intramolecular atomic interactions in halogen-substituted trinitromethanes. Physical Chemistry Chemical Physics, 2014, 16, 16780-16789.	1.3	20
174	Ring-annelated corannulenes as fullerene receptors. A DFT-D study. RSC Advances, 2014, 4, 29826-29833.	1.7	33
175	Complementary optical and neutron vibrational spectroscopy study of bromanilic acid: 2,3,5,6-tetramethylpyrazine (1:1) cocrystal. Vibrational Spectroscopy, 2014, 75, 26-38.	1.2	12
176	Experimental and Computational Study of Counterintuitive ClO <sub>4</sub> <sup>–</sup> A·A·A·ClO <sub>4</sub> <sup>–</sup> Interactions and the Interplay between le <sup>+</sup> –le and Anion·A·le <sup>+</sup> Interactions. Crystal Growth and Design, 2014, 14, 5812-5821.	1.4	113
177	Origin of the Spectral Shifts among the Early Intermediates of the Rhodopsin Photocycle. Journal of the American Chemical Society, 2014, 136, 3842-3851.	6.6	42
178	Physical Nature of Interactions in Zn <sup>II</sup> Complexes with 2,2â $\in$ 2-Bipyridyl: Quantum Theory of Atoms in Molecules (QTAIM), Interacting Quantum Atoms (IQA), Noncovalent Interactions (NCI), and Extended Transition State Coupled with Natural Orbitals for Chemical Valence (ETS-NOCV) Comparative Studies. Journal of Physical Chemistry A, 2014, 118, 623-637.	1.1	81
179	Labelling Herceptin with a novel oxaliplatin derivative: a computational approach towards the selective drug delivery. Journal of Molecular Modeling, 2014, 20, 2401.	0.8	24
180	Substituted Corannulenes and Sumanenes as Fullerene Receptors. A Dispersion-Corrected Density Functional Theory Study. Journal of Physical Chemistry A, 2014, 118, 9521-9528.	1.1	49
181	Does intramolecular hydrogen bond play a key role in the stereochemistry of α- and β-d-glucose?. Carbohydrate Research, 2014, 396, 9-13.	1.1	30
182	Molecule VI: Sulfonimide or Sulfonamide?. Crystal Growth and Design, 2014, 14, 3704-3710.	1.4	16
183	Longâ€Range Effects in Anion–΀ Interactions: Their Crucial Role in the Inhibition Mechanism of <i>Mycobacterium Tuberculosis</i> Malate Synthase. Chemistry - A European Journal, 2014, 20, 6985-6990.	1.7	35

#	Article	IF	CITATIONS
184	Interaction of Anions with Substituted Buckybowls. The Anion's Nature and Solvent Effects. Journal of Physical Chemistry A, 2014, 118, 6112-6124.	1.1	12
185	Experimental and theoretical investigations of the self-association of oxaliplatin. Physical Chemistry Chemical Physics, 2014, 16, 14688-14698.	1.3	10
186	Chemical Assignment of Symmetry-Adapted Perturbation Theory Interaction Energy Components: The Functional-Group SAPT Partition. Journal of Chemical Theory and Computation, 2014, 10, 4417-4431.	2.3	101
187	Complexation of Ni(ClO <sub>4</sub> ) <sub>2</sub> and Mg(ClO <sub>4</sub> ) <sub>2</sub> with 3-Hydroxyflavone in Acetonitrile Medium: Conductometric, Spectroscopic, and Quantum Chemical Investigation. Journal of Physical Chemistry B, 2014, 118, 12251-12262.	1.2	8
188	A combined experimental and theoretical study of the supramolecular self-assembly of Cu(II) malonate complex assisted by various weak forces and water dimer. Journal of Solid State Chemistry, 2014, 220, 149-156.	1.4	22
189	DFT-steric-based energy decomposition analysis of intermolecular interactions. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	43
190	Why Does Substitution of Thymine by 6-Ethynylpyridone Increase the Thermostability of DNA Double Helices?. Journal of Physical Chemistry B, 2014, 118, 6586-6596.	1.2	17
191	Simultaneous Visualization of Covalent and Noncovalent Interactions Using Regions of Density Overlap. Journal of Chemical Theory and Computation, 2014, 10, 3745-3756.	2.3	177
192	Nonclassical CHâ^Ï€ Supramolecular Interactions in Artemisinic Acid Favor a Single Conformation, Yielding High Diastereoselectivity in the Reduction with Diazene. Journal of Organic Chemistry, 2014, 79, 5939-5947.	1.7	13
194	Wave Function and Density Functional Theory Studies of Dihydrogen Complexes. Journal of Chemical Theory and Computation, 2014, 10, 3151-3162.	2.3	23
195	The effect of fluorine substitution in alcohol–amine complexes. Physical Chemistry Chemical Physics, 2014, 16, 22882-22891.	1.3	61
196	Toward Efficient Drug Delivery through Suitably Prepared Metal–Organic Frameworks: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 8885-8890.	1.5	37
197	Experimental and Solid-State Computational Study of Structural and Dynamic Properties in the Equilibrium Form of Temazepam. Journal of Physical Chemistry B, 2014, 118, 6670-6679.	1.2	5
198	A study on the versatility of metallacycles in host–guest chemistry: Interactions in halide-centered hexanuclear copper(ii) pyrazolate complexes. Physical Chemistry Chemical Physics, 2014, 16, 13103.	1.3	16
199	Complexes between hypohalous acids and phosphine derivatives. Pnicogen bond versus halogen bond versus hydrogen bond. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 271-277.	2.0	33
200	Computational study of anion recognition based on tetrel and hydrogen bonding interaction by calix[4]pyrrole derivatives. Computational and Theoretical Chemistry, 2014, 1038, 67-70.	1.1	67
201	Reversible dimerization of viologen radicals covalently linked to a calixarene platform: Experimental and theoretical aspects. Comptes Rendus Chimie, 2014, 17, 505-511.	0.2	20
202	Unusual outcome of the thermolytic condensation of diazoarylmethanes with a [tricarbonyl(η6-2-p-tolyl)chromium]2-oxazolyl chelate of tetracarbonylrhenium. Journal of Organometallic Chemistry, 2014, 751, 754-759.	0.8	13

#	Article	IF	Citations
203	A new turn in codon–anticodon selection through halogen bonds. Physical Chemistry Chemical Physics, 2014, 16, 7430.	1.3	17
204	A Ï $f$ -hole interaction with radical species as electron donors: does single-electron tetrel bonding exist?. Physical Chemistry Chemical Physics, 2014, 16, 11617-11625.	1.3	113
205	Tuning the Halogen/Hydrogen Bond Competition: A Spectroscopic and Conceptual DFT Study of Some Model Complexes Involving CHF <sub>2</sub> 1. Chemistry - A European Journal, 2014, 20, 8433-8443.	1.7	50
206	Interaction of aromatic units of amino acids with guanidinium cation: The interplay of π···π, XH··€, and M <sup>+</sup> ···π contacts. Journal of Computational Chemistry, 2014, 35, 1290-1301.	1.5	15
207	Density Functional Study of Interactions between Fluorinated Cyclohexanes and Arenes. Helvetica Chimica Acta, 2014, 97, 797-807.	1.0	4
208	Mechanistic Insights on the Stereoselective Nucleophilic 1,2-Addition to Sulfinyl Imines. Journal of Organic Chemistry, 2014, 79, 2514-2521.	1.7	18
209	A theoretical probe on the non-covalent interactions of sulfadoxine drug with pi-acceptors. Journal of Molecular Structure, 2014, 1074, 157-167.	1.8	6
210	Is there an attractive interaction between two methyl groups?. Chemical Physics Letters, 2014, 608, 90-94.	1.2	7
211	A Carbeneâ€Rich but Carbonylâ€Poor [Ir <sub>6</sub> (IMe) <sub>8</sub> (CO) <sub>2</sub> H <sub>14</sub> ] <sup>2+</sup> Polyhydride Cluster as a Deactivation Product from Catalytic Glycerol Dehydrogenation. Angewandte Chemie - International Edition, 2014, 53, 12808-12811.	7.2	42
213	A Carbeneâ€Rich but Carbonylâ€Poor [Ir <sub>6</sub> (IMe) <sub>8</sub> (CO) <sub>2</sub> H <sub>14</sub> ] <sup>2+</sup> Polyhydride Cluster as a Deactivation Product from Catalytic Glycerol Dehydrogenation. Angewandte Chemie, 2014, 126, 13022-13025.	1.6	9
214	Hydrosilylation Induced by N→Si Intramolecular Coordination: Spontaneous Transformation of Organosilanes into 1â€Azaâ€Siloleâ€Type Molecules in the Absence of a Catalyst. Chemistry - A European Journal, 2014, 20, 2542-2550.	1.7	23
215	Influence of Fluorination on the Conformational Properties and Hydrogenâ€Bond Acidity of Benzyl Alcohol Derivatives. Chemistry - A European Journal, 2015, 21, 11462-11474.	1.7	25
216	A new smoothing function to introduce long-range electrostatic effects in QM/MM calculations. Journal of Chemical Physics, 2015, 143, 044103.	1.2	21
217	Electron density analysis of large (molecular and periodic) systems: A parallel implementation. Journal of Computational Chemistry, 2015, 36, n/a-n/a.	1.5	30
218	London Dispersion in Molecular Chemistry—Reconsidering Steric Effects. Angewandte Chemie - International Edition, 2015, 54, 12274-12296.	7.2	719
219	Attraction or Repulsion? London Dispersion Forces Control Azobenzene Switches. Angewandte Chemie - International Edition, 2015, 54, 13436-13439.	7.2	84
221	Fiber Surfaces: Generalizing Isosurfaces to Bivariate Data. Computer Graphics Forum, 2015, 34, 241-250.	1.8	45
222	Hexahalogenated and their mixed benzene derivatives as prototypes for the understanding of halogen···halogen intramolecular interactions: New insights from combined DFT, QTAIMâ€; and RDGâ€based NCI analyses. Journal of Computational Chemistry, 2015, 36, 2328-2343.	1.5	20

#	Article	IF	CITATIONS
223	London'sche Dispersionswechselwirkungen in der Molekülchemie – eine Neubetrachtung sterischer Effekte. Angewandte Chemie, 2015, 127, 12446-12471.	1.6	197
224	Folding Patterns in a Family of Oligoamide Foldamers. Chemistry - A European Journal, 2015, 21, 9493-9504.	1.7	16
225	Stimuliâ€Responsive Frustrated Lewisâ€Pairâ€Type Reactivity of a Tungsten Iminoazaphosphiridine Complex. Chemistry - A European Journal, 2015, 21, 9650-9655.	1.7	20
226	Intramolecular OHâ‹â‹â‹Fluorine Hydrogen Bonding in Saturated, Acyclic Fluorohydrins: The γâ€Fluoropropanol Motif. Chemistry - A European Journal, 2015, 21, 17808-17816.	1.7	41
227	On the Importance of CH/Ï€ and CHâ‹â‹HC Interactions in the Solid State Structure of 15â€Lipox Inhibitors Based on Eugenol Derivatives. ChemPhysChem, 2015, 16, 2260-2266.	/genase 1.0	17
228	A Rationally Designed Thymidineâ€Based Selfâ€Assembled Monolayer on a Cold Electrode for Electroanalytical Applications. Chemistry - an Asian Journal, 2015, 10, 1554-1560.	1.7	4
229	Interaction of Iron II Complexes with B-DNA. Insights from Molecular Modeling, Spectroscopy, and Cellular Biology. Frontiers in Chemistry, 2015, 3, 67.	1.8	9
230	An exceptional functionalization of doped fullerene observed via theoretical studies on the interactions of sulfur-doped fullerenes with halogens and halides. RSC Advances, 2015, 5, 55227-55237.	1.7	14
231	Solubility prediction of bio-oil derived chemicals in aqueous media by Localized Molecular Orbital-Energy Decomposition Analysis (LMO-EDA) and COSMO-RS predictions. Computational and Theoretical Chemistry, 2015, 1067, 48-59.	1.1	3
232	Mechanisms and stereoselectivities of the Rh( <scp>i</scp> )-catalyzed carbenoid carbon insertion reaction of benzocyclobutenol with diazoester. Organic and Biomolecular Chemistry, 2015, 13, 6587-6597.	1.5	36
233	Dual functions of Lewis acid and base of Se in F2C=Se and their interplay in F2CSe•••••••HX of Molecular Modeling, 2015, 21, 157.	Journal	4
234	Experimental and theoretical evaluation of trans-3-halo-2-hydroxy-tetrahydropyran conformational preferences. Beyond anomeric interaction. RSC Advances, 2015, 5, 35412-35420.	1.7	14
235	Inverted Carbon Geometries: Challenges to Experiment and Theory. Journal of Organic Chemistry, 2015, 80, 6520-6524.	1.7	22
236	Cucurbit[6]uril: A Possible Host for Noble Gas Atoms. Journal of Physical Chemistry B, 2015, 119, 10962-10974.	1.2	50
237	Non-covalent interactions in ionic liquid ion pairs and ion pair dimers: a quantum chemical calculation analysis. Physical Chemistry Chemical Physics, 2015, 17, 16846-16857.	1.3	59
238	Development of asymmetrical near infrared squaraines with large Stokes shift. RSC Advances, 2015, 5, 106868-106876.	1.7	15
239	Molecular recognition of thiaclopride by Aplysia californica AChBP: new insights from a computational investigation. Journal of Computer-Aided Molecular Design, 2015, 29, 1151-1167.	1.3	8
240	Predicting the relative binding affinity of mineralocorticoid receptor antagonists by density functional methods. Journal of Computer-Aided Molecular Design, 2015, 29, 1109-1122.	1.3	7

#	Article	IF	CITATIONS
241	Effect of 2-Substituents on Allyl-Supported Precatalysts for the Suzuki–Miyaura Reaction: Relating Catalytic Efficiency to the Stability of Palladium(I) Bridging Allyl Dimers. Organometallics, 2015, 34, 381-394.	1.1	38
242	Hydrogen–hydrogen bonding: The current density perspective. Journal of Computational Chemistry, 2015, 36, 707-716.	1.5	19
243	Origins of Asymmetric Phosphazene Organocatalysis: Computations Reveal a Common Mechanism for Nitro- and Phospho-Aldol Additions. Journal of Organic Chemistry, 2015, 80, 2756-2766.	1.7	30
244	Electronic Structure and Noncovalent Interactions within Ion–Radical Complexes of <i>N</i> -(2-Furylmethyl)aniline Molecular Ions. Journal of Physical Chemistry A, 2015, 119, 2098-2110.	1.1	4
245	How do organic gold compounds and organic halogen molecules interact? Comparison with hydrogen bonds. RSC Advances, 2015, 5, 12488-12497.	1.7	18
246	Efficient Organocatalyst Supported on a Simple Ionic Liquid as a Recoverable System for the Asymmetric Diels–Alder Reaction in the Presence of Water. ChemCatChem, 2015, 7, 830-835.	1.8	32
247	Unprecedented Ring–Ring Interconversion of N,P,C age Ligands. Chemistry - A European Journal, 2015, 21, 3727-3735.	1.7	17
248	Enantioselective Organocatalytic Reduction of βâ€₹rifluoromethyl Nitroalkenes: An Efficient Strategy for the Synthesis of Chiral βâ€₹rifluoromethyl Amines. Chemistry - A European Journal, 2015, 21, 3589-3595.	1.7	35
249	Role of Noncovalent Interactions in Vanadium Tellurite Chain Connectivities. Inorganic Chemistry, 2015, 54, 694-703.	1.9	14
250	Tailoring buckybowls for fullerene recognition. A dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2015, 17, 6233-6241.	1.3	22
251	Entasis through Hook-and-Loop Fastening in a Glycoligand with Cumulative Weak Forces Stabilizing Cu <sup>I</sup> . Journal of the American Chemical Society, 2015, 137, 1141-1146.	6.6	23
252	Conceptual Quantum Chemical Analysis of Bonding and Noncovalent Interactions in the Formation of Frustrated Lewis Pairs. Chemistry - A European Journal, 2015, 21, 5510-5519.	1.7	30
253	Interplay between Cation–π and Coinageâ€Metal–Oxygen Interactions: An Ab Initio Study and Cambridge Structural Database Survey. ChemPhysChem, 2015, 16, 1008-1016.	1.0	9
254	The Missing Entry in the Agostic–Anagostic Series: Rh(I)–η <sup>1</sup> -C Interactions in P(CH)P Pincer Complexes. Inorganic Chemistry, 2015, 54, 2960-2969.	1.9	46
255	Fullerene recognition with molecular tweezers made up of efficient buckybowls: a dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2015, 17, 13206-13214.	1.3	26
256	A computational study on the steric effects of naphthenic moieties on aggregation interactions of nonconventional petroleum constituents. Journal of Physical Organic Chemistry, 2015, 28, 234-241.	0.9	4
257	An anion induced multisignaling probe for Hg <sup>2+</sup> and its application for fish kidney and liver tissue imaging studies. Dalton Transactions, 2015, 44, 13186-13195.	1.6	20
258	DensToolKit: A comprehensive open-source package for analyzing the electron density and its derivative scalar and vector fields. Computer Physics Communications, 2015, 196, 362-371.	3.0	22

#	Article	IF	CITATIONS
259	An energy decomposition analysis study for intramolecular non-covalent interaction. Chemical Physics Letters, 2015, 635, 250-256.	1.2	22
260	Effective utilization of noncovalent interaction descriptor in BX3–Lewis base complexes: A determination of adduct/van der Waals complexes and reassessment of the BX3 acid strength order. Chemical Physics Letters, 2015, 636, 117-120.	1.2	6
261	Intramolecular and intermolecular bromineâ< polyfluoroarene interactions: The crystal structure of bis{κC-1-(2,3,5,6-tetrafluoropyridyl)-3-benzylimidazolin-2-ylidene}tetrabromodimercury. Journal of Fluorine Chemistry, 2015, 178, 178-182.	0.9	1
262	Elucidation of Photoisomerization-Related Structural Changes in an Acrylamide-Bridged Binaphthalene–Diazene Macrocyclic Chiroptical Switch by Experimental Electronic Circular Dichroism Spectra Simulation: Role of Dispersion Corrections. Journal of Physical Chemistry A, 2015, 119. 8588-8598.	1.1	3
263	Stabilization of an Electron-Unsaturated Pd(I)–Pd(I) Unit by Double Hemichelation. Organometallics, 2015, 34, 3055-3064.	1.1	18
264	Observation of novel oxygenâ< oxygen interaction in supramolecular assembly of cobalt( <scp>iii</scp> ) Schiff base complexes: a combined experimental and computational study. RSC Advances, 2015, 5, 73028-73039.	1.7	36
265	A <scp>DFT</scp> study on the insertion of <scp>CO</scp> <sub>2</sub> into styrene oxide catalyzed by 1â€butylâ€3â€methylâ€imidazolium bromide ionic liquid. Journal of Computational Chemistry, 2015, 36, 1322-1333.	1.5	31
266	The relationship between the strength of hydrogen bonding and spin crossover behaviour in a series of iron( <scp>iii</scp> ) Schiff base complexes. Dalton Transactions, 2015, 44, 4474-4484.	1.6	53
267	Multiple active zones in hybrid QM/MM molecular dynamics simulations for large biomolecular systems. Physical Chemistry Chemical Physics, 2015, 17, 9959-9972.	1.3	11
268	A Chemically Meaningful Measure of Electron Localization. Journal of Chemical Theory and Computation, 2015, 11, 3617-3628.	2.3	14
269	Structural evolution of (Au <sub>2</sub> S) <sub>n</sub> (n = 1–8) clusters from first principles global optimization. RSC Advances, 2015, 5, 62543-62550.	1.7	17
270	Electrochemical and Fluorescent Ferrocene-Imidazole-Based Dyads as Ion-Pair Receptors for Divalent Metal Cations and Oxoanions. Inorganic Chemistry, 2015, 54, 7461-7473.	1.9	40
271	Understanding the thermal dehydrochlorination reaction of 1-chlorohexane. Revealing the driving bonding pattern at the planar catalytic reaction center. RSC Advances, 2015, 5, 62946-62956.	1.7	9
272	Synthesis and Reactions of 3d Metal Complexes with the Bulky Alkoxide Ligand [OC <sup><i>t</i></sup> Bu <sub>2</sub> Ph]. Inorganic Chemistry, 2015, 54, 5624-5633.	1.9	32
273	Metal containing cryptands as hosts for anions: evaluation of Cu( <scp>i</scp> )⋯X and π⋯X interactions in halide–tricopper( <scp>i</scp> ) complexes through relativistic DFT calculations. Physical Chemistry Chemical Physics, 2015, 17, 18677-18683.	1.3	11
274	On the interaction between the imidazolium cation and aromatic amino acids. A computational study. Organic and Biomolecular Chemistry, 2015, 13, 7961-7972.	1.5	13
275	Examining the compatibility of collagen and a polythiophene derivative for the preparation of bioactive platforms. RSC Advances, 2015, 5, 9189-9203.	1.7	7
276	Noncovalent interactions determine the conformation of aurophilic complexes with 2-mercapto-4-methyl-5-thiazoleacetic acid ligands. Dalton Transactions, 2015, 44, 13641-13650.	1.6	5

#	Article	IF	CITATIONS
277	Crystallization-Driven Multicomponent Encapsulation of Coulombically Repulsive Guests. Crystal Growth and Design, 2015, 15, 3525-3531.	1.4	5
278	Reconciling Experiment and Theory in the Use of Aryl-Extended Calix[4]pyrrole Receptors for the Experimental Quantification of Chlorideâ€″Ï€ Interactions in Solution. International Journal of Molecular Sciences, 2015, 16, 8934-8948.	1.8	10
279	Critical Assessment of the Strength of Hydrogen Bonds between the Sulfur Atom of Methionine/Cysteine and Backbone Amides in Proteins. Journal of Physical Chemistry Letters, 2015, 6, 1385-1389.	2.1	76
280	Evidence for Terminal Phosphinidene Oxide Complexes in O,P,C-Cage Complex Formation: Rearrangement of Oxaphosphirane Complexes. Organometallics, 2015, 34, 2676-2682.	1.1	16
281	Organic fluorines as halogen bond donors: Theoretical study and crystallographic evidence. International Journal of Quantum Chemistry, 2015, 115, 884-890.	1.0	13
282	Determination of the molecular structure of gaseous proline by electron diffraction, supported by microwave and quantum chemical data. Structural Chemistry, 2015, 26, 1489-1500.	1.0	8
283	Understanding the azeotropic diethyl carbonate–water mixture by structural and energetic characterization of DEC(H2O) n heteroclusters. Journal of Molecular Modeling, 2015, 21, 93.	0.8	3
284	Improving As( <scp>iii</scp> ) adsorption on graphene based surfaces: impact of chemical doping. Physical Chemistry Chemical Physics, 2015, 17, 12056-12064.	1.3	49
285	Understanding Bond Formation in Polar One-Step Reactions. Topological Analyses of the Reaction between Nitrones and Lithium Ynolates. Journal of Organic Chemistry, 2015, 80, 4076-4083.	1.7	32
286	IQA-embedded fragment attributed molecular system energy change in exploring intramolecular interactions. Computational and Theoretical Chemistry, 2015, 1066, 62-75.	1.1	26
287	Structure and dynamics of the fibronectin-III domains of Aplysia californica cell adhesion molecules. Physical Chemistry Chemical Physics, 2015, 17, 9634-9643.	1.3	2
288	Ionic liquids as solvents of polar and non-polar solutes: affinity and coordination. Physical Chemistry Chemical Physics, 2015, 17, 14588-14597.	1.3	17
289	Hydrogen Bonds Involving Sulfur: New Insights from ab Initio Calculations and Gas Phase Laser Spectroscopy. Challenges and Advances in Computational Chemistry and Physics, 2015, , 15-45.	0.6	40
290	Dynamics of the chemical bond: inter- and intra-molecular hydrogen bond. Faraday Discussions, 2015, 177, 51-64.	1.6	24
291	Experimental and theoretical evaluation on the conformational behavior of <scp>l</scp> -aspartic acid dimethyl ester and its N-acetylated derivative. RSC Advances, 2015, 5, 18013-18024.	1.7	7
292	Secondary bonding networks in small (HgS)n clusters: A theoretical investigation. Computational and Theoretical Chemistry, 2015, 1060, 36-42.	1.1	4
293	Hydrogen bonding and π–π interactions in imidazolium-chloride ionic liquid clusters. Physical Chemistry Chemical Physics, 2015, 17, 14437-14453.	1.3	113
294	Origin of Chemoselectivity in N-Heterocyclic Carbene Catalyzed Cross-Benzoin Reactions: DFT and Experimental Insights. Journal of Organic Chemistry, 2015, 80, 3597-3610.	1.7	57

#	Article	IF	CITATIONS
295	Meta-Hybrid Density Functional Theory Study of Adsorption of Imidazolium- and Ammonium-Based Ionic Liquids on Graphene Sheet. Journal of Physical Chemistry C, 2015, 119, 7095-7108.	1.5	68
296	Toward an Understanding of Diamond sp <sup>2</sup> -Defects with Unsaturated Diamondoid Oligomer Models. Journal of the American Chemical Society, 2015, 137, 6577-6586.	6.6	19
297	Expanding Lone Pair···Ĩ€ Interactions to Nonaromatic Systems and Nitrogen Bases: Complexes of C <sub>2</sub> F <sub>3</sub> X (X = F, Cl, Br, I) and TMA- <i>d</i> <sub>9</sub> . Journal of Physical Chemistry A, 2015, 119, 5597-5606.	1.1	30
298	Dihydrogen Bond Intermediated Alcoholysis of Dimethylamine–Borane in Nonaqueous Media. Journal of Physical Chemistry A, 2015, 119, 3853-3868.	1.1	22
299	Properties of Ammonium Ion–Water Clusters: Analyses of Structure Evolution, Noncovalent Interactions, and Temperature and Humidity Effects. Journal of Physical Chemistry A, 2015, 119, 3035-3047.	1.1	25
300	DFT Study of the Energetic and Noncovalent Interactions between Imidazolium Ionic Liquids and Hydrofluoric Acid. Journal of Physical Chemistry B, 2015, 119, 5002-5009.	1.2	26
301	Hydrothermal synthesis, X-ray structure and DFT and magnetic studies of a (H <sub>2</sub> SiW <sub>12</sub> O <sub>40</sub> ) <sup>2â^²</sup> based one-dimensional linear coordination polymer. Dalton Transactions, 2015, 44, 8824-8832.	1.6	34
302	Two new copper and nickel complexes of pyridine-2,6-dicarboxylic acid N-oxide and their proton transferred salts: Solid state and DFT insights. Inorganica Chimica Acta, 2015, 438, 135-145.	1.2	16
303	Theoretical study on interactions of fluorinated organomercurials with arene and gold fragments. Physical Chemistry Chemical Physics, 2015, 17, 26417-26428.	1.3	5
304	Microhydration of Protonated Nα-Acetylhistidine: A Theoretical Approach. Journal of Physical Chemistry B, 2015, 119, 11527-11539.	1.2	5
305	Structural-topological preferences and protonation sequence of aliphatic polyamines: a theoretical case study of tetramine trien. Journal of Molecular Modeling, 2015, 21, 162.	0.8	5
306	Gel-assisted crystallization of [Ir <sub>4</sub> (IMe) <sub>7</sub> (CO)H <sub>10</sub> ] <sup>2+</sup> and [Ir <sub>4</sub> (IMe) <sub>8</sub> H <sub>9</sub> ] <sup>3+</sup> clusters derived from catalytic glycerol dehydrogenation. Dalton Transactions, 2015, 44, 18403-18410.	1.6	20
307	Role of the cation formal charge in cation–΀ interaction. A survey involving the [2.2.2]paracyclophane host from relativistic DFT calculations. New Journal of Chemistry, 2015, 39, 9963-9968.	1.4	23
308	Electron Density Distribution of Urea in Co-crystals with Rigid and Flexible Dicarboxylic Acids. Crystal Growth and Design, 2015, 15, 5578-5592.	1.4	13
309	Understanding the high reactivity of carbonyl compounds towards nucleophilic carbenoid intermediates generated from carbene isocyanides. RSC Advances, 2015, 5, 84797-84809.	1.7	21
310	α- and α′-Lithiation–Electrophile Trapping of <i>N</i> -Thiopivaloyl and <i>N</i> - <i>tert</i> -Butoxythiocarbonyl α-Substituted Azetidines: Rationalization of the Regiodivergence Using NMR and Computation. Journal of Organic Chemistry, 2015, 80, 9838-9846.	1.7	21
311	Toward Prediction of the Chemistry in Ionic Liquids: An Accurate Computation of Absolute p <i>K</i> <sub>a</sub> Values of Benzoic Acids and Benzenethiols. Journal of Organic Chemistry, 2015, 80, 8997-9006.	1.7	19
312	Intramolecular Hydrogen Bonding in Methyl Lactate. Journal of Physical Chemistry A, 2015, 119, 9692-9702.	1.1	29

#	Article	IF	CITATIONS
313	Halogen bonding interactions in ion pairs versus conventional charge-assisted and neutral halogen bonds: a theoretical study based on imidazolium species. RSC Advances, 2015, 5, 74284-74294.	1.7	20
314	Approaching the double-faceted nature of the CX bond in halobenzenes with a bifunctional probe. Chemical Physics Letters, 2015, 637, 51-57.	1.2	2
315	Synthesis, structure, magnetic property and self-assembly of two double end-on azide bridged ferromagnetic nickel(II) complexes with distinct bidentate blocking ligands: A combined experimental and theoretical study. Polyhedron, 2015, 101, 257-269.	1.0	17
316	Unusual bonding modes of perfluorobenzene in its polymeric (dimeric, trimeric and tetrameric) forms: entirely negative fluorine interacting cooperatively with entirely negative fluorine. Physical Chemistry Chemical Physics, 2015, 17, 31624-31645.	1.3	34
317	Is there an intramolecular hydrogen bond in 2-halophenols? A theoretical and spectroscopic investigation. Physical Chemistry Chemical Physics, 2015, 17, 25151-25159.	1.3	30
318	Weak intramolecular and intermolecular hydrogen bonding of benzyl alcohol, 2-phenylethanol and 2-phenylethylamine in the adsorption on graphitized thermal carbon black. Physical Chemistry Chemical Physics, 2015, 17, 24282-24293.	1.3	11
319	DFT study of 1-butyl-3-methylimidazolium salicylate: a third-generation ionic liquid. Journal of Molecular Modeling, 2015, 21, 246.	0.8	16
320	Probing molecular interactions underlying imidazolium and pyridinium based ionic liquids. Journal of Molecular Liquids, 2015, 212, 885-899.	2.3	11
321	Origin of Stereodivergence in Cooperative Asymmetric Catalysis with Simultaneous Involvement of Two Chiral Catalysts. Journal of the American Chemical Society, 2015, 137, 15712-15722.	6.6	99
322	Non-classical CHâ <sup>,-</sup> O hydrogen-bond determining the regio- and stereoselectivity in the [3 + 2] cycloaddition reaction of (Z)-C-phenyl-N-methylnitrone with dimethyl 2-benzylidenecyclopropane-1,1-dicarboxylate. A topological electron-density study. RSC Advances, 2015, 5. 99299-99311.	1.7	36
323	Effect of ï€â€"ï€ interaction in Bergman cyclisation. Physical Chemistry Chemical Physics, 2015, 17, 29793-29802.	1.3	3
324	Assessment of hydrophobic interactions and their contributions through the analysis of the methane dimer. Journal of Computational Chemistry, 2015, 36, 361-375.	1.5	16
325	Intra-residue interactions in proteins: interplay between serine or cysteine side chains and backbone conformations, revealed by laser spectroscopy of isolated model peptides. Physical Chemistry Chemical Physics, 2015, 17, 2169-2178.	1.3	31
326	[2.2.2]Paracyclophane, preference for η <sup>6</sup> or η <sup>18</sup> coordination mode including Ag( <scp>i</scp> ) and Sn( <scp>ii</scp> ): a survey into the cationâ€''i€ interaction nature through relativistic DFT calculations. RSC Advances, 2015, 5, 7803-7811.	1.7	25
327	NCI analysis of the interaction cationâ<ï€ in complexes with molecular bowls derived from fullerene. Computational and Theoretical Chemistry, 2015, 1053, 123-129.	1.1	8
328	Competition of C(sp <sup>2</sup> )–X···O Halogen Bonding and Lone Pair···π Interactions: Cryospectroscopic Study of the Complexes of C <sub>2</sub> F <sub>3</sub> X (X = F, Cl, Br, and I) and Dimethyl Ether. Journal of Physical Chemistry A, 2015, 119, 2502-2516.	1.1	32
329	Revealing halogen bonding interactions with anomeric systems: An ab initio quantum chemical studies. Journal of Molecular Graphics and Modelling, 2015, 55, 123-133.	1.3	9
330	Superstable Palladium(0) Complex as an Air―and Thermostable Catalyst for Suzuki Coupling Reactions. European Journal of Organic Chemistry, 2015, 2015, 60-66.	1.2	19

#	Article	IF	CITATIONS
331	Electron density analysis of aromatic complexes in excited electronic states: The benzene and naphthalene excimers. Computational and Theoretical Chemistry, 2015, 1053, 220-228.	1.1	24
332	Intervalence charge transfer across noncovalent interactions on vinyl silyl bridged biferrocenyl compounds. Computational and Theoretical Chemistry, 2015, 1053, 281-288.	1.1	5
333	Molecular structure and conformations of caramboxin, a natural neurotoxin from the star fruit: A computational study. Journal of Molecular Structure, 2015, 1079, 274-280.	1.8	2
334	Evaluating common QTAIM and NCI interpretations of the electron density concentration through IQA interaction energies and 1D cross-sections of the electron and deformation density distributions. Computational and Theoretical Chemistry, 2015, 1053, 60-76.	1.1	50
335	Chemical structure and reactivity by means of quantum chemical topology analysis. Computational and Theoretical Chemistry, 2015, 1053, 17-30.	1.1	62
336	Scrutinizing ion-ï€ and ion-ïƒ interactions using the noncovalent index and energy decomposition analysis. Computational and Theoretical Chemistry, 2015, 1053, 150-164.	1.1	9
337	A view of covalent and ionic bonding from Maximum Probability Domains. Computational and Theoretical Chemistry, 2015, 1053, 142-149.	1.1	23
338	Effects of the CO2 Guest Molecule on the sI Clathrate Hydrate Structure. Materials, 2016, 9, 777.	1.3	33
339	Why p-OMe- and p-Cl-β-Methylphenethylamines Display Distinct Activities upon MAO-B Binding. PLoS ONE, 2016, 11, e0154989.	1.1	7
340	Evaluating the Free Energies of Solvation and Electronic Structures of Lithiumâ€lon Battery Electrolytes. ChemPhysChem, 2016, 17, 2916-2930.	1.0	36
342	Die Kationâ€Ï€â€Wechselwirkung in der Katalyse mit niedermolekularen Verbindungen. Angewandte Chemie, 2016, 128, 12784-12814.	1.6	49
343	The Conformational Map of Volatile Anesthetics: Enflurane Revisited. Chemistry - A European Journal, 2016, 22, 9804-9811.	1.7	4
344	Neutral iodotriazoles as scaffolds for stable halogen-bonded assemblies in solution. Chemical Science, 2016, 7, 6422-6428.	3.7	33
345	Unsaturation in binuclear heterometallic carbonyls: the cyclopentadienyliron manganese carbonyl CpFeMn(CO) <sub>n</sub> system as a hybrid of the Cp <sub>2</sub> Fe <sub>2</sub> (CO) <sub>n</sub> and Mn <sub>2</sub> (CO) <sub>n</sub> systems. New Journal of Chemistry, 2016, 40, 7482-7492.	1.4	4
346	The Cation–π Interaction in Smallâ€Molecule Catalysis. Angewandte Chemie - International Edition, 2016, 55, 12596-12624.	7.2	199
347	αâ€Fluoroâ€ <i>o</i> â€cresols: The Key Role of Intramolecular Hydrogen Bonding in Conformational Preference and Hydrogenâ€Bond Acidity. ChemPhysChem, 2016, 17, 2702-2709.	1.0	12
348	Association of symmetrical alkane diols with pyridine: DFT/GIAO calculation of <sup>1</sup> H NMR chemical shifts. Magnetic Resonance in Chemistry, 2016, 54, 805-814.	1.1	12
349	Computational Characterization of the Origin of Selectivity in Cycloaddition Reactions Catalyzed by Phosphoric Acid Derivatives. Chemistry - an Asian Journal, 2016, 11, 411-416.	1.7	25

#	Article	IF	CITATIONS
350	Molecular simulations and density functional theory calculations of bromine in clathrate hydrate phases. Journal of Chemical Physics, 2016, 144, 044501.	1.2	13
351	Analysis of transition state stabilization by non-covalent interactions in the Houk–List model of organocatalyzed intermolecular Aldol additions using functional-group symmetry-adapted perturbation theory. Physical Chemistry Chemical Physics, 2016, 18, 10297-10308.	1.3	23
352	A theoretical quantum study of the intramolecular interactions and chemical reactivity of polymorphs A and B of famotidine in the gas, DMSO, and aqueous phases. Computational and Theoretical Chemistry, 2016, 1075, 54-62.	1.1	6
353	Resolving the Physical Origin of Octahedral Tilting in Halide Perovskites. Chemistry of Materials, 2016, 28, 4259-4266.	3.2	211
354	The role of nonbonding interactions and the presence of fluoride on the conformational isomerism of 1,2-ethanediol. Chemical Physics, 2016, 473, 17-23.	0.9	11
355	NCI concept as a powerful tool to investigate the origin of Diels–Alder reaction accelerating inside the self-assembled softball nanoreactor. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 85, 237-246.	0.9	2
356	Molecular structure, hydrogen-bonding patterns and topological analysis (QTAIM and NCI) of 5-methoxy-2-nitroaniline and 5-methoxy-2-nitroaniline with 2-amino-5-nitropyridine (1:1) co-crystal. Journal of Molecular Structure, 2016, 1119, 505-516.	1.8	18
357	Deprotonation of Al <sub>2</sub> Me <sub>6</sub> by Sterically Bulky NHCs: Scope, Rationale through DFT Studies, and Application in the Methylenation of Carbonyl Substrates. Organometallics, 2016, 35, 1726-1734.	1.1	8
358	Complex modes of bonding: NCI/ELI-D vs. DORI surface analyses of hapticities and hydrogen–hydrogen contacts in zincocene related compounds. Chemical Physics Letters, 2016, 651, 172-177.	1.2	28
359	CdS Nanoparticles Fabricated from the Single-Source Precursor [Cd{Et <sub>2</sub> NC(S)NP(S)(O <i>i</i> Pr) <sub>2</sub> } <sub>2</sub> ]: In Depth Experimental and Theoretical Studies. Crystal Growth and Design, 2016, 16, 3287-3296.	1.4	8
360	Probing the ATP-induced conformational flexibility of the PcrA helicase protein using molecular dynamics simulation. Journal of Molecular Modeling, 2016, 22, 54.	0.8	7
361	The interaction of Pd clusters with the bulk and layered two-dimensional Silicalite-1 supports. Catalysis Today, 2016, 277, 108-117.	2.2	2
362	A new tetranuclear copper(I) cluster of 1,3-bis(4-bromophenyl)triazene ligand: Synthesis, characterization, structural and computational studies. Inorganica Chimica Acta, 2016, 446, 32-40.	1.2	5
363	Nature, Strength, and Cooperativity of the Hydrogen-Bonding Network in α-Chitin. Biomacromolecules, 2016, 17, 996-1003.	2.6	57
364	Alkali Ion Incorporation into V <sub>2</sub> O <sub>5</sub> : a Noncovalent Interactions Analysis. Journal of Physical Chemistry C, 2016, 120, 4259-4265.	1.5	17
365	Origin of the Catalytic Effects of Molecular Iodine: A Computational Analysis. ACS Catalysis, 2016, 6, 3203-3212.	5.5	108
366	Size evolution and ligand effects on the structures and stability of (AuL) <sub>n</sub> (L = Cl, SH,) Tj ETQq0 0 0 2016, 6, 4705-4712.	rgBT /Over 1.7	lock 10 Tf 50 27
367	Cooperative Asymmetric Catalysis by N-Heterocyclic Carbenes and BrÃ,nsted Acid in Î <sup>3</sup> -Lactam Formation: Insights into Mechanism and Stereoselectivity. ACS Catalysis, 2016, 6, 3118-3126.	5.5	58

#	Article	IF	CITATIONS
368	"Conformational lock―via unusual intramolecular C–F⋯Oî€C and C–H⋯Cl–C parallel dipoles observe in situ cryocrystallized liquids. Chemical Communications, 2016, 52, 7225-7228.	d_in 2:2	31
369	Transition State Models for Understanding the Origin of Chiral Induction in Asymmetric Catalysis. Accounts of Chemical Research, 2016, 49, 1019-1028.	7.6	118
370	Exploration of unconventional π–hole and C–Hâ <h–c a="" cd(<scp="" in="" interactions="" of="" supramolecular="" trinuclear="" types="">ii) and a heteronuclear Cd(<scp>ii</scp>)–Ni(<scp>ii</scp>) complex and experimental evidence for preferential site selection of the ligand by 3d and 4d metal ions. RSC Advances, 2016, 6, 39376-39386.</h–c>	1.7	13
371	Completing the Heterocubane Family [Cp*AlE] <sub>4</sub> (E = O, S, Se, and Te) by Selective Oxygenation and Sulfuration of [Cp*Al] <sub>4</sub> : Density Functional Theory Calculations of [Cp*AlE] <sub>4</sub> and Reactivity of [Cp*AlO] <sub>4</sub> toward Hydrolysis. Inorganic Chemistry. 2016. 55. 4915-4923.	1.9	38
372	[3+2] Cycloaddition reaction of 1H-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl acrylate: A DFT study. Computational and Theoretical Chemistry, 2016, 1087, 36-47.	1.1	2
373	Non-covalent stacking interactions directing the structural and photophysical features of mono- and dinuclear cyclometalated palladium( <scp>ii</scp> ) complexes. Dalton Transactions, 2016, 45, 8601-8613.	1.6	9
374	Three cation-templated Cu( <scp>i</scp> ) self-assemblies: synthesis, structures, and photocatalytic properties. New Journal of Chemistry, 2016, 40, 6086-6092.	1.4	25
375	A Complete NCI Perspective: From New Bonds to Reactivity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 491-527.	0.6	24
376	The nature of inter- and intramolecular interactions in F2OXe…HX (X= F, Cl, Br, I) complexes. Journal of Molecular Modeling, 2016, 22, 119.	0.8	1
377	Nuclear spin hyperpolarization with ansa-aminoboranes: a metal-free perspective for parahydrogen-induced polarization. Physical Chemistry Chemical Physics, 2016, 18, 27784-27795.	1.3	34
378	Reevaluating the Stability and Prevalence of Conglomerates: Implications for Preferential Crystallization. Crystal Growth and Design, 2016, 16, 6055-6059.	1.4	29
379	Energetic Materials Trends in 5―and 6â€Membered Cyclic Peroxides Containing Hydroperoxy and Hydroxy Substituents. European Journal of Inorganic Chemistry, 2016, 2016, 5036-5043.	1.0	8
380	Theoretical Investigation of Oxidative Cleavage of Cholesterol by Dual O2 Activation and Sulfide Reduction. Australian Journal of Chemistry, 2016, 69, 933.	0.5	2
381	Hydrogen Bonding and Stability of Hybrid Organic–Inorganic Perovskites. ChemSusChem, 2016, 9, 2648-2655.	3.6	109
382	Protonation State of MnFe and FeFe Cofactors in a Ligand-Binding Oxidase Revealed by X-ray Absorption, Emission, and Vibrational Spectroscopy and QM/MM Calculations. Inorganic Chemistry, 2016, 55, 9869-9885.	1.9	15
383	Lone pairâ<ï€ interactions involving carbonyl ï€-systems: Experimental and theoretical study of the complexes of COF2 and COFCI with dimethyl ether. Chemical Physics, 2016, 476, 1-8.	0.9	5
384	An intermolecular pyrene excimer in the pyrene-labeled N-thiophosphorylated thiourea and its nickel( <scp>ii</scp> ) complex. Inorganic Chemistry Frontiers, 2016, 3, 1419-1431.	3.0	14
385	Characterization of Nâ⊄O non-covalent interactions involving σ-holes: "electrostatics―or "dispersion― Physical Chemistry Chemical Physics, 2016, 18, 29946-29954.	1.3	14

#	Article	IF	CITATIONS
386	Molecular dynamics simulation and quantum chemical studies on the investigation of aluminum nitride nanotube as phosgene gas sensor. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 86, 305-322.	0.9	37
387	Experimental and Theoretical AIM and NCI Index Study of Substituted Arene Tricarbonyl Complexes of Chromium(0). ChemistrySelect, 2016, 1, 5014-5018.	0.7	6
388	An MEDT study of the carbenoid-type [3 + 2] cycloaddition reactions of nitrile ylides with electron-deficient chiral oxazolidinones. Organic and Biomolecular Chemistry, 2016, 14, 10427-10436.	1.5	15
389	Characterization of the nucleation precursor (H <sub>2</sub> SO <sub>4</sub> –(CH <sub>3</sub> ) <sub>2</sub> NH) complex: intra-cluster interactions and atmospheric relevance. RSC Advances, 2016, 6, 5824-5836.	1.7	9
390	Catalytic aspects of metallophthalocyanines adsorbed on gold-electrode. Theoretical exploration of the binding nature role. Physical Chemistry Chemical Physics, 2016, 18, 29516-29525.	1.3	10
391	Tiara-like Complexes acting as Iodine Encapsulating Agents: The Role of M···I Interactions in [M(μ-SCH <sub>2</sub> CO <sub>2</sub> Me) <sub>2</sub> ] <sub>8</sub> âŠ,I <sub>2</sub> (M = Ni, Pd, Pt) Inclusion Compounds. Journal of Physical Chemistry C, 2016, 120, 23441-23448.	1.5	9
392	Infrared spectrum of the cold ortho-fluorinated protonated neurotransmitter 2-phenylethylamine: competition between NH <sup>+</sup> â<ï€ and NH <sup>+</sup> â<ïF interactions. Physical Chemistry Chemical Physics, 2016, 18, 26980-26989.	1.3	10
393	A benchmark for the non-covalent interaction (NCI) index or… is it really all in the geometry?. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	124
394	Why are sec-alkylperoxyl bimolecular self-reactions orders of magnitude faster than the analogous reactions of tert-alkylperoxyls? The unanticipated role of CH hydrogen bond donation. Physical Chemistry Chemical Physics, 2016, 18, 23673-23679.	1.3	56
395	Bonding, Luminescence, Metallophilicity in Linear Au <sub>3</sub> and Au <sub>2</sub> Ag Chains Stabilized by Rigid Diphosphanyl NHC Ligands. Inorganic Chemistry, 2016, 55, 8527-8542.	1.9	47
396	In Silico Design of Halogen-Bonding-Based Organocatalyst for Diels–Alder Reaction, Claisen Rearrangement, and Cope-Type Hydroamination. Journal of Organic Chemistry, 2016, 81, 7459-7470.	1.7	43
397	Synthesis of malhamensilipin A exploiting iterative epoxidation/chlorination: experimental and computational analysis of epoxide-derived chloronium ions. Chemical Science, 2016, 7, 7040-7049.	3.7	13
398	Interactions affecting <sup>1</sup> J <sub>C–F</sub> SSCCs in neutral and ionic 2-, 3- and 4-fluoro-substituted piperidines: normal and reverse fluorine Perlin-like effect. RSC Advances, 2016, 6, 74598-74603.	1.7	11
399	Orthoâ€7 bound to the activeâ€site gorge of free and <scp>OP</scp> onjugated acetylcholinesterase: Cation–π interactions. Biopolymers, 2016, 105, 10-20.	1.2	5
400	Modulating the strength of tetrel bonding through beryllium bonding. Journal of Molecular Modeling, 2016, 22, 192.	0.8	28
401	Synthesis, spectral and structural characterization and computational studies of rhenium(I)-tricarbonyl nitrito complexes of 2,2′-bipyridine and 2,9-dimethylphenanthroline ligands: Ĩ€-Accepting character of the diimine ligands. Inorganica Chimica Acta, 2016, 453, 357-368.	1.2	18
402	Acid–Base Formalism Extended to Excited State for O–H···S Hydrogen Bonding Interaction. Journal of Physical Chemistry A, 2016, 120, 6902-6916.	1.1	9
403	Improving the Property–Function Tuning Range of Thiophene Materials via Facile Synthesis of Oligo/Polythiopheneâ€Sâ€Oxides and Mixed Oligo/Polythiopheneâ€Sâ€Oxides/Oligo/Polythiopheneâ€S,Sâ€Dioxi Advanced Functional Materials, 2016, 26, 6970-6984.	d <i>ø</i> s8	25

#	Article	IF	CITATIONS
404	Noncovalent interactions between the second coordination sphere and the active site of [NiFeSe] hydrogenase. RSC Advances, 2016, 6, 81636-81646.	1.7	1
406	Guanidine-catalyzed asymmetric Strecker reaction: modes of activation and origin of stereoselectivity. Canadian Journal of Chemistry, 2016, 94, 1099-1108.	0.6	5
407	Theoretical study of intermolecular interactions in crystalline arene–perhaloarene adducts in terms of the electron density. RSC Advances, 2016, 6, 77301-77309.	1.7	11
408	Boronâ€Boron Oneâ€Electron Sigma Bonds versus Bâ€Xâ€B Bridged Structures. Chemistry - A European Journal, 2016, 22, 13697-13704.	1.7	13
409	Azaâ€Michael Reactions of Isatin Imines: Deeper Insight and Origin of the Stereoselectivity. ChemCatChem, 2016, 8, 2961-2967.	1.8	3
410	A halogen bond does not dictate the conformational preferences of cis-1,3-disubstituted cyclohexanes. Organic and Biomolecular Chemistry, 2016, 14, 8610-8614.	1.5	2
411	Revisiting sulfur H-bonds in proteins: The example of peroxiredoxin AhpE. Scientific Reports, 2016, 6, 30369.	1.6	52
412	The explicit examination of the magnetic states of electrides. Physical Chemistry Chemical Physics, 2016, 18, 27326-27335.	1.3	16
413	Modulation in π⋨I€, cationâ<¯I€ and C–H⋯H–C interactions varying the counter anions in square planar nickel(II) Schiff base complexes: A combined experimental and theoretical study. Polyhedron, 2016, 119, 451-459.	1.0	9
414	Dinitrogen-Facilitated Reversible Formation of a Si–H Bond in a Pincer-Supported Ni Complex. Organometallics, 2016, 35, 3154-3162.	1.1	33
415	Intramolecular C–H···H–C Contacts in Diheteroaryl Ketones and Thioketones: A Theoretical Analysis. Bulletin of the Chemical Society of Japan, 2016, 89, 92-102.	2.0	12
416	Solvatomorphism in (Z)-4-fluoro-N′-(3-fluorophenyl)benzimidamide: the role of intermolecular O–H⋯F interaction. CrystEngComm, 2016, 18, 8291-8300.	1.3	4
417	Multiscale Treatment for the Molecular Mechanism of a Diels–Alder Reaction in Solution: A QM/MM-MD Study. Journal of Chemical Theory and Computation, 2016, 12, 4735-4742.	2.3	14
418	Computing organic stereoselectivity – from concepts to quantitative calculations and predictions. Chemical Society Reviews, 2016, 45, 6093-6107.	18.7	175
419	Intramolecular Hydrogen Bonding in Substituted Aminoalcohols. Journal of Physical Chemistry A, 2016, 120, 6371-6378.	1.1	40
421	Multiple Weak C–H Intramolecular Hydrogen Bonding as an Aid to Minimizing Bond Rotation Flexibility. Crystal Growth and Design, 2016, 16, 4934-4942.	1.4	7
422	How the mechanism of a [3 + 2] cycloaddition reaction involving a stabilized N-lithiated azomethine ylide toward a π-deficient alkene is changed to stepwise by solvent polarity? What is the origin of its regio- and endo stereospecificity? A DFT study using NBO, QTAIM, and NCI analyses. RSC Advances, 2016, 6, 75299-75314.	1.7	20
423	A combined experimental and theoretical study on two new dinuclear cadmium(II) Schiff base complexes with selenocyanate-κ-Se. Inorganica Chimica Acta, 2016, 453, 51-61.	1.2	11

#	Article	IF	CITATIONS
424	Effect of Peptide Sequences on Supramolecular Interactions of Naphthaleneimide/Tripeptide Conjugates. Langmuir, 2016, 32, 7630-7638.	1.6	31
425	Beryllium subphthalocyanines self-assembling properties. Canadian Journal of Chemistry, 2016, 94, 1015-1021.	0.6	3
426	A silver coordination cage assembled from [Ag <sub>2</sub> (bis(isoxazolyl)) <sub>3</sub> ]: DFT approach to the binding forces within the host–guest interactions. RSC Advances, 2016, 6, 103346-103356.	1.7	4
427	Mechanism and Stereoselectivity in an Asymmetric N-Heterocyclic Carbene-Catalyzed Carbon–Carbon Bond Activation Reaction. Organic Letters, 2016, 18, 5932-5935.	2.4	27
428	BrÃ,nsted Acid Catalysis—Structural Preferences and Mobility in Imine/Phosphoric Acid Complexes. Journal of the American Chemical Society, 2016, 138, 15965-15971.	6.6	40
429	Carbon-nanorings ([10]CPP and [6]CPPA) as fullerene (C60 and C70) receptors: a comprehensive dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2016, 18, 31670-31679.	1.3	26
430	Visualizing and Quantifying Interactions in the Excited State. Chemistry - A European Journal, 2016, 22, 18442-18449.	1.7	22
431	Investigation of allosteric modulation mechanism of metabotropic glutamate receptor 1 by molecular dynamics simulations, free energy and weak interaction analysis. Scientific Reports, 2016, 6, 21763.	1.6	23
432	Nitrogen induced phosphorene formation on the boron phosphide (111) surface: a density functional theory study. RSC Advances, 2016, 6, 108621-108626.	1.7	2
433	Role of Dispersion in Metallophilic Hg···M Interactions (M = Cu, Ag, Au) within Coinage Metal Complexes of Bis(6-diphenylphosphinoacenaphth-5-yl)mercury. Inorganic Chemistry, 2016, 55, 11513-11521.	1.9	24
434	Steric and electric field driven distortions in aromatic molecules: spontaneous and non-spontaneous symmetry breaking. Physical Chemistry Chemical Physics, 2016, 18, 31160-31167.	1.3	23
435	How to Twist, Split and Warp a σ-Hole with Hypervalent Halogens. Journal of Physical Chemistry A, 2016, 120, 9431-9445.	1.1	45
436	Effects of Aromatic Fluorine Substitution on Protonated Neurotransmitters: The Case of 2â€Phenylethylamine. Chemistry - A European Journal, 2016, 22, 8124-8136.	1.7	13
437	Structure and Stability Studies of Pharmacologically Relevant <i>S</i> -Nitrosothiols: A Theoretical Approach. Journal of Physical Chemistry A, 2016, 120, 4191-4200.	1.1	18
438	Cooperativity of intermolecular hydrogen bonds in microsolvated DMSO and DMF clusters: a DFT, AIM, and NCI analysis. Journal of Molecular Modeling, 2016, 22, 151.	0.8	40
439	A novel method for copper( <scp>ii</scp> ) mediated region-selective bromination of aromatic rings under mild conditions. RSC Advances, 2016, 6, 61214-61220.	1.7	20
440	Alteration of intermolecular interactions between units of asphaltene dimers exposed to an amide-enriched modifier. RSC Advances, 2016, 6, 53477-53492.	1.7	36
441	Pentanidium-Catalyzed Asymmetric Phase-Transfer Conjugate Addition: Prediction of Stereoselectivity via DFT Calculations and Docking Sampling of Transition States, and Origin of Stereoselectivity. Australian Journal of Chemistry, 2016, 69, 983.	0.5	10

#	Article	IF	CITATIONS
442	Encapsulation of small gas molecules and rare gas atoms inside the octa acid cavitand. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	29
443	Evidence of a Donor–Acceptor (Ir–H)→SiR <sub>3</sub> Interaction in a Trapped Ir(III) Silane Catalytic Intermediate. Organometallics, 2016, 35, 2207-2223.	1.1	40
444	Selectivity in Gas Adsorption by Molecular Cucurbit[6]uril. Journal of Physical Chemistry C, 2016, 120, 13911-13921.	1.5	49
445	The Mechanism of Acceptorless Amine Double Dehydrogenation by <i>N,N,N</i> -Amide Ruthenium(II) Hydrides: A Combined Experimental and Computational Study. ACS Catalysis, 2016, 6, 4799-4813.	5.5	56
446	Conciliatory Inductive Model Explaining the Origin of Changes in the η <sup>2</sup> -SiH Bond Length Caused by Presence of Strongly Electronegative Atoms X (X = F, Cl) in Cp(OC) <sub>2</sub> Mn[η <sup>2</sup> -H(SiH <sub>3â€"<i>n</i></sub> X <sub><i>n</i></sub> )] ( <i>n</i> ) =)	Tj ETQq0 (	) OrgBT /Ove
447	Hydrogen and Dihydrogen Bonds in the Reactions of Metal Hydrides. Chemical Reviews, 2016, 116, 8545-8587.	23.0	181
448	Interacting quantum fragmentsâ€rooted preorganizedâ€interacting fragments attributed relative molecular stability of the Be <sup>II</sup> complexes of nitrilotriacetic acid and nitrilotriâ€3â€propionic acid. Journal of Computational Chemistry, 2016, 37, 1373-1387.	1.5	11
449	Intriguing E…E' bonding in [Nap(EPh)(E'Ph)] <sup>•+</sup> (E, E'=O, S, Se, Te). International Journal of Quantum Chemistry, 2016, 116, 1090-1096.	1.0	3
450	Adaptive quantum mechanics/molecular mechanics methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 369-385.	6.2	51
451	Electride: from computational characterization to theoretical design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 430-440.	6.2	41
452	A novel nanostructured supramolecular hydrogel self-assembled from tetraphenylethylene-capped dipeptides. Soft Matter, 2016, 12, 6347-6351.	1.2	25
453	Understanding the stereoselectivity in BrÃ,nsted acid catalysed Povarov reactions generating cis/trans CF <sub>3</sub> -substituted tetrahydroquinolines: a DFT study. RSC Advances, 2016, 6, 17064-17073.	1.7	17
454	Can an entirely negative fluorine in a molecule, viz. perfluorobenzene, interact attractively with the entirely negative site(s) on another molecule(s)? Like liking like!. RSC Advances, 2016, 6, 19098-19110.	1.7	42
455	Unravelling Protein–DNA Interactions at Molecular Level: A DFT and NCI Study. Journal of Chemical Theory and Computation, 2016, 12, 523-534.	2.3	35
456	Theoretical investigation of the backbone··À·Ï€ and π··ÄE stacking interactions in substituted-benzene  3-methyl-2′-deoxyadenosine: a perspective to the DNA repair. Molecular Physics, 2016, 114, 774-783.	0.8	3
457	Molecular structures of two tetrodotoxin analogs containing a monooxa-hydrocarbon cage: A computational study. Journal of Molecular Structure, 2016, 1106, 407-415.	1.8	2
458	How strong are the metallocene–metallocene interactions? Cases of ferrocene, ruthenocene, and osmocene. Physical Chemistry Chemical Physics, 2016, 18, 550-556.	1.3	34
459	Compositional control of pore geometry in multivariate metal–organic frameworks: an experimental and computational study. Dalton Transactions, 2016, 45, 4316-4326.	1.6	19

#	Article	IF	CITATIONS
460	Preferred Geometries and Energies of Sulfur–Sulfur Interactions in Crystal Structures. Crystal Growth and Design, 2016, 16, 632-639.	1.4	54
461	N-Heterocyclic Carbene (NHC)-Catalyzed sp <sup>3</sup> β-C–H Activation of Saturated Carbonyl Compounds: Mechanism, Role of NHC, and Origin of Stereoselectivity. ACS Catalysis, 2016, 6, 279-289.	5.5	99
462	Bidirectional Interaction of Alanine with Sulfuric Acid in the Presence of Water and the Atmospheric Implication. Journal of Physical Chemistry A, 2016, 120, 2357-2371.	1.1	29
463	First principles study on the structural evolution and properties of (MCl) <sub>n</sub> (n = 1–12, M =) Tj ETQo	1 1 0.784 1.7	314 rgBT /0
464	Lone pair···π interactions involving an aromatic π-system: Complexes of hexafluorobenzene with dimethyl ether and trimethylamine. Chemical Physics Letters, 2016, 647, 26-30.	1.2	8
465	Surface on Surface. Survey of the Monolayer Gold–Graphene Interaction from Au <sub>12</sub> and PAH via Relativistic DFT Calculations. Journal of Physical Chemistry C, 2016, 120, 7358-7364.	1.5	12
466	Modeling Polymorphic Molecular Crystals with Electronic Structure Theory. Chemical Reviews, 2016, 116, 5567-5613.	23.0	294
467	An Evolving Insight into Chiral H-Bond Catalyzed Aza-Henry Reactions: A Cooperative Role for Noncovalent Attractive Interactions Unveiled by Density Functional Theory. Journal of Organic Chemistry, 2016, 81, 3286-3295.	1.7	10
468	Theoretical assessment of phosgene adsorption behavior onto pristine, Al- and Ga-doped B12N12 and B16N16 nanoclusters. Computational Materials Science, 2016, 118, 155-171.	1.4	45
469	Conformational flexibility of PPII-helix: A density functional theory study. Chemical Physics Letters, 2016, 651, 109-113.	1.2	3
470	Novel Di- and Trinuclear Palladium Complexes Supported by <i>N</i> , <i>N</i> ′-Diphosphanyl NHC Ligands and <i>N</i> , <i>N</i> ′-Diphosphanylimidazolium Palladium, Gold, and Mixed-Metal Copper–Gold Complexes. Inorganic Chemistry, 2016, 55, 1219-1229.	1.9	32
471	CO <sub>2</sub> Absorption Using Fluorine Functionalized Ionic Liquids: Interplay of Hydrogen and Ïf-Hole Interactions. Journal of Physical Chemistry A, 2016, 120, 1243-1260.	1.1	21
472	Development of bis(arylimino)acenaphthene (BIAN) copper complexes as visible light harvesters for potential photovoltaic applications. Inorganic Chemistry Frontiers, 2016, 3, 651-662.	3.0	41
473	Electron conjugation versus π–π repulsion in substituted benzenes: why the carbon–nitrogen bond in nitrobenzene is longer than in aniline. Physical Chemistry Chemical Physics, 2016, 18, 11821-11828.	1.3	33
474	Understanding the molecular switching properties of octaphyrins. Physical Chemistry Chemical Physics, 2016, 18, 11885-11900.	1.3	29
475	On the nature of the stabilisation of the Eâ<ï€ pnicogen bond in the SbCl <sub>3</sub> â<ītoluene complex. Chemical Communications, 2016, 52, 3500-3503.	2.2	39
476	Understanding the Mechanism of the Lewis Acid Promoted [3 + 2] Cycloaddition of Propargylic Alcohol and α-Oxo Ketene Dithioacetals. Journal of Organic Chemistry, 2016, 81, 1989-1997.	1.7	13
477	Atropisomerism about Aryl–C(sp3) Bonds: Conformational Behavior of Substituted Phenylcyclohexanes in Solution. Journal of Organic Chemistry, 2016, 81, 2372-2382.	1.7	13

#	Article	IF	CITATIONS
478	Insights into metal–ligand and metal–metal interaction in coinage metal triangles. Insights of d10-d10, d10-d8 and d8-d8 contacts from [Au3I (CH3N COCH3)3] (n= 2, 4, 6) via relativistic DFT calculations. Chemical Physics Letters, 2016, 651, 34-38.	1.2	5
479	Strain Control: Reversible H <sub>2</sub> Activation and H <sub>2</sub> /D <sub>2</sub> Exchange in Pt Complexes. Inorganic Chemistry, 2016, 55, 3023-3029.	1.9	18
480	Investigation of the molecular structure, electronic properties, AIM, NBO, NMR and NQR parameters for the interaction of Sc, Ga and Mg-doped (6,0) aluminum nitride nanotubes with COCl2 gas by DFT study. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 84, 99-114.	0.9	34
481	Revealing Stepwise Mechanisms in Dipolar Cycloaddition Reactions: Computational Study of the Reaction between Nitrones and Isocyanates. Journal of Organic Chemistry, 2016, 81, 673-680.	1.7	25
482	Influence of sumanene modifications with boron and nitrogen atoms to its hydrogen adsorption properties. Physical Chemistry Chemical Physics, 2016, 18, 2859-2870.	1.3	42
483	Theoretical exploration of seleno and tellurophenols as promising alternatives to sulfur ligands for anchoring to gold (111) materials. RSC Advances, 2016, 6, 4458-4468.	1.7	8
484	Exploiting the cyclodextrins ability for antioxidants encapsulation: A computational approach to carnosol and carnosic acid embedding. Computational and Theoretical Chemistry, 2016, 1077, 65-73.	1.1	21
485	Urea hydration from dielectric relaxation spectroscopy: old findings confirmed, new insights gained. Physical Chemistry Chemical Physics, 2016, 18, 2597-2607.	1.3	30
486	Recognition of halides and Y-shaped oxoanions by carbonylchromium-based urea-like molecules: A theoretical analysis of hydrogen bonding modes. Journal of Molecular Graphics and Modelling, 2016, 64, 1-10.	1.3	3
487	London Dispersion Decisively Contributes to the Thermodynamic Stability of Bulky NHC-Coordinated Main Group Compounds. Journal of Chemical Theory and Computation, 2016, 12, 231-237.	2.3	74
488	New Pd( <scp>ii</scp> ) hemichelates devoid of incipient bridging COâ‹ <sup>-</sup> Pd interactions. Dalton Transactions, 2016, 45, 607-617.	1.6	9
489	Synthesis, crystal structure and DFT calculations of bis(1,3-diazinane-2-thione-κS)dicyanido disilver(I), [{Ag(Diaz)2}{Ag(CN)2}]. Polyhedron, 2016, 110, 299-304.	1.0	8
490	Synthesis and structure of new 1-cyanoacetyl-4-arylsemicarbazide derivatives with potential anticancer activity. Journal of Molecular Structure, 2016, 1104, 24-32.	1.8	6
491	Intramolecular halogen bonds in 1,2-aryldiyne molecules: a theoretical study. Structural Chemistry, 2016, 27, 907-917.	1.0	6
492	Study of noncovalent interactions of end-caped sulfur-doped carbon nanotubes using DFT, QTAIM, NBO and NCI calculations. Structural Chemistry, 2016, 27, 739-751.	1.0	23
493	Structure and stability of clusters of $\hat{l}^2$ -alanine in the gas phase: importance of the nature of intermolecular interactions. Physical Chemistry Chemical Physics, 2017, 19, 5465-5476.	1.3	6
494	Trapping of organophosphorus chemical nerve agents by pillar[5]arene: A DFT, AIM, NCI and EDA analysis. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2017, 87, 207-218.	0.9	37
495	Cooperative Binding in a Phosphine Oxide-Based Halogen Bonded Dimer Drives Supramolecular Oligomerization. Journal of Organic Chemistry, 2017, 82, 1986-1995.	1.7	24

#	Article	IF	CITATIONS
496	Pseudohalides regulated diverse helicity in copper(II) coordination polymers derived from a bis(aminoethoxy) ligand. Polyhedron, 2017, 124, 262-274.	1.0	3
497	Spectroscopic Evidences for Strong Hydrogen Bonds with Selenomethionine in Proteins. Journal of Physical Chemistry Letters, 2017, 8, 794-800.	2.1	49
498	A computational study on the role of noncovalent interactions in the stability of polymer/graphene nanocomposites. Journal of Molecular Modeling, 2017, 23, 43.	0.8	22
499	Alternative Route Toward Nitrones: Experimental and Theoretical Findings. Journal of Organic Chemistry, 2017, 82, 1666-1675.	1.7	5
500	The mechanism of an asymmetric ring-opening reaction of epoxide with amine catalyzed by a metal–organic framework: insights from combined quantum mechanics and molecular mechanics calculations. Dalton Transactions, 2017, 46, 3470-3481.	1.6	35
501	Weak Supramolecular Interactions Governing Parallel and Antiparallel DNA Quadruplexes: Insights from Large cale Quantum Mechanics Analysis of Experimentally Derived Models. Chemistry - A European Journal, 2017, 23, 5573-5584.	1.7	9
502	Tuning the HOMO–LUMO Energy Gap of Small Diamondoids Using Inverse Molecular Design. Journal of Chemical Theory and Computation, 2017, 13, 1351-1365.	2.3	42
503	Insights into the Diels–Alder Reaction between 3-Vinylindoles and Methyleneindolinone without and with the Assistance of Hydrogen-Bonding Catalyst Bisthiourea: Mechanism, Origin of Stereoselectivity, and Role of Catalyst. Journal of Organic Chemistry, 2017, 82, 3046-3061.	1.7	30
504	Theoretical insights into the ultrafast excited-state intramolecular proton transfer (ESIPT) mechanism in a series of amide-based N Hâ<̄N hydrogen-bonding compounds. Organic Electronics, 2017, 45, 1-8.	1.4	42
505	Efficient and Selective Hydrosilylation of Secondary and Tertiary Amides Catalyzed by an Iridium(III) Metallacycle: Development and Mechanistic Investigation. ChemCatChem, 2017, 9, 2009-2017.	1.8	28
506	A DFT study on lignin dissolution in imidazolium-based ionic liquids. RSC Advances, 2017, 7, 12670-12681.	1.7	100
507	Nature of the interaction between ammonia derivatives and carbon disulfide. A theoretical investigation. International Journal of Quantum Chemistry, 2017, 117, e25369.	1.0	12
508	Characterizing magnesium bonds: main features of a non-covalent interaction. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	21
509	Electronic and Steric Manipulation of the Preagostic Interaction in Isoquinoline Complexes of Rh <sup>I</sup> . European Journal of Inorganic Chemistry, 2017, 2017, 2255-2264.	1.0	16
510	On the Importance of Ï€â€Hole Beryllium Bonds: Theoretical Study and Biological Implications. Chemistry - A European Journal, 2017, 23, 5375-5380.	1.7	19
511	Insight into the role of weak interaction played in the fixation of CO 2 catalyzed by the amino-functionalized imidazolium-based ionic liquids. Journal of CO2 Utilization, 2017, 18, 156-163.	3.3	39
512	How does the global electron density transfer diminish activation energies in polar cycloaddition reactions? A Molecular Electron Density Theory study. Tetrahedron, 2017, 73, 1718-1724.	1.0	65
513	Halogen-Bond-Based Molecular Self-Assembly on Graphene Surface: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 4451-4461.	1.5	17

#	Article	IF	CITATIONS
514	Revealing the Intermolecular Interactions of Asphaltene Dimers by Quantum Chemical Calculations. Energy & Fuels, 2017, 31, 2488-2495.	2.5	59
515	Mapping the Trajectory of Nucleophilic Substitution at Silicon Using a <i>peri</i> â€Substituted Acenaphthyl Scaffold. Chemistry - A European Journal, 2017, 23, 10568-10579.	1.7	27
516	Selective Oxidation and Functionalization of 6-Diphenylphosphinoacenaphthyl-5-tellurenyl Species 6-Ph <sub>2</sub> P-Ace-5-TeX (X = Mes, Cl, O <sub>3</sub> SCF <sub>3</sub> ). Various Types of P–E···Te(II,IV) Bonding Situations (E = O, S, Se). Organometallics, 2017, 36, 1566-1579.	1.1	18
517	Theoretical insights on a series of difluoramino group-based energetic molecules. Journal of Physical Organic Chemistry, 2017, 30, e3704.	0.9	5
518	Exploring the reversal of enantioselectivity on a zinc-dependent alcohol dehydrogenase. Organic and Biomolecular Chemistry, 2017, 15, 4122-4129.	1.5	36
519	QTAIM and NCI analysis of intermolecular interactions in steroid ligands binding a cytochrome P450 enzyme – Beyond the most obvious interactions. Computational and Theoretical Chemistry, 2017, 1111, 40-49.	1.1	24
520	Origin of Remarkably Different Acidity of Hydroxycoumarins—Joint Experimental and Theoretical Studies. Journal of Physical Chemistry B, 2017, 121, 4554-4561.	1.2	29
521	Kinetic Energy Density as a Predictor of Hydrogen-Bonded OH-Stretching Frequencies. Journal of Physical Chemistry A, 2017, 121, 3452-3460.	1.1	25
522	Crystal Structure Analysis and Topological Study of Non-covalent Interactions in 2,2-Biimidazole:Salicylic Acid 2:1 Co-crystal. Journal of Chemical Crystallography, 2017, 47, 47-58.	0.5	8
523	Effect of Lewis acid bulkiness on the stereoselectivity of Diels–Alder reactions between acyclic dienes and α,β-enals. Organic Chemistry Frontiers, 2017, 4, 1390-1399.	2.3	29
524	Effect of Fluorination on the Competition of Halogen Bonding and Hydrogen Bonding: Complexes of Fluoroiodomethane with Dimethyl Ether and Trimethylamine. Journal of Physical Chemistry A, 2017, 121, 4180-4188.	1.1	16
525	London Dispersion Enables the Shortest Intermolecular Hydrocarbon H···H Contact. Journal of the American Chemical Society, 2017, 139, 7428-7431.	6.6	126
526	Trapping CO <sub>2</sub> by Adduct Formation with Nitrogen Heterocyclic Carbenes (NHCs): A Theoretical Study. Chemistry - A European Journal, 2017, 23, 10604-10609.	1.7	45
527	Electronic structure and rearrangements of anionic [ClMg(η2-O2C)]â^' and [ClMg(η2-CO2)]â^' complexes: a quantum chemical topology study. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	8
528	Mercurophilic interactions: a theoretical study on the importance of ligands. Physical Chemistry Chemical Physics, 2017, 19, 11645-11654.	1.3	31
529	An Orbitalâ€Overlap Complement to Atomic Partial Charge. Angewandte Chemie - International Edition, 2017, 56, 6878-6881.	7.2	8
530	The inhibition process of HIV-1 integrase by diketoacids molecules: Understanding the factors governing the better efficiency of dolutegravir. Biochemical and Biophysical Research Communications, 2017, 488, 433-438.	1.0	4
531	Importance of Dispersion on the Stability of the Concave-Bound CpM (M = Fe, Ru, Os) Complexes of Sumanene. Organometallics, 2017, 36, 2036-2041.	1.1	4

#	Article	IF	CITATIONS
532	Dissection of H-bonding interactions in a glycolic acid–water dimer. Physical Chemistry Chemical Physics, 2017, 19, 14238-14247.	1.3	8
533	Introducing topology to assess the synchronicity of organic reactions. Dual reactivity of oximes with alkenes as a case study. Organic Chemistry Frontiers, 2017, 4, 1541-1554.	2.3	22
534	An Orbitalâ€Overlap Complement to Atomic Partial Charge. Angewandte Chemie, 2017, 129, 6982-6985.	1.6	0
535	Insights into Frustrated and Regular peri -Substituted (Ace-)Naphthylaminoboranes and (Ace-)Naphthylphosphinoboranes. European Journal of Inorganic Chemistry, 2017, 2017, 3302-3311.	1.0	12
536	A cleft type receptor which combines an oxyanion hole with electrostatic interactions. Organic and Biomolecular Chemistry, 2017, 15, 4571-4578.	1.5	3
537	Decrypting Transition States by Light: Photoisomerization as a Mechanistic Tool in BrÃ,nsted Acid Catalysis. Journal of the American Chemical Society, 2017, 139, 6752-6760.	6.6	31
538	Steric interactions controlling the <i>syn</i> diastereofacial selectivity in the [3Â+Â2] cycloaddition reaction between acetonitrile oxide and 7-oxanorborn-5-en-2-ones: A molecular electron density theory study. Journal of Physical Organic Chemistry, 2017, 30, e3710.	0.9	23
539	Tuning the electronic properties of monolayer and bilayer transition metal dichalcogenide compounds under direct out-of-plane compression. Physical Chemistry Chemical Physics, 2017, 19, 13333-13340.	1.3	20
540	Thermodynamic cycles of the alkali metal–ligand complexes central to electride formation. Physical Chemistry Chemical Physics, 2017, 19, 12816-12825.	1.3	7
541	Occurrence of 3D isostructurality in fluorinated phenyl benzamidines. CrystEngComm, 2017, 19, 47-63.	1.3	16
542	Understanding the reaction mechanism of the Lewis acid (MgBr2)-catalysed [3+2] cycloaddition reaction between C-methoxycarbonyl nitrone and 2-propen-1-ol: a DFT study. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	9
543	Does Z′ equal 1 or 2? Enhanced powder NMR crystallography verification of a disordered room temperature crystal structure of a p38 inhibitor for chronic obstructive pulmonary disease. Physical Chemistry Chemical Physics, 2017, 19, 16650-16661.	1.3	25
544	trans–cis C–Pd–C rearrangement in hemichelates. Dalton Transactions, 2017, 46, 8125-8137.	1.6	9
545	A DFT computational study on the molecular mechanism of reaction between pyridinium salts and ï€-deficient ethylenes: Why furan derivatives are formed instead of feasible cyclopropane derivatives and [3 + 2] cycloadducts?. Computational and Theoretical Chemistry, 2017, 1114, 87-100.	1.1	6
546	Quantum Chemical Modeling of Hydrogen Bonding in Ionic Liquids. Topics in Current Chemistry, 2017, 375, 59.	3.0	48
547	The Mouse in a Trap: Observation of a C(sp3)–F···F–C(sp3) Interaction in a Discrete CFC Pair by the Crystal Sponge Method. Crystal Growth and Design, 2017, 17, 3611-3615.	1.4	13
548	New insights into human farnesyl pyrophosphate synthase inhibition by second-generation bisphosphonate drugs. Journal of Computer-Aided Molecular Design, 2017, 31, 675-688.	1.3	3
549	Ï€-Backbonding and non-covalent interactions in the JohnPhos and polyfluorothiolate complexes of gold( <scp>i</scp> ). Dalton Transactions, 2017, 46, 12456-12465.	1.6	9

#	Article	IF	CITATIONS
550	Accurately extracting the signature of intermolecular interactions present in the NCI plot of the reduced density gradient versus electron density. Physical Chemistry Chemical Physics, 2017, 19, 17928-17936.	1.3	1,068
551	Does Confinement Always Lead to Thermodynamically and/or Kinetically Favorable Reactions? A Case Study using Diels–Alder Reactions within ExBox <sup>+4</sup> and CB[7]. ChemPhysChem, 2017, 18, 2162-2170.	1.0	24
552	Visualization of weak interactions between quantum dot and graphene in hybrid materials. Scientific Reports, 2017, 7, 417.	1.6	11
553	New Rutheniumâ€Based Probes for Selective Gâ€Quadruplex Targeting. Chemistry - A European Journal, 2017, 23, 11872-11880.	1.7	32
554	Theoretical analysis of the binding of iron(III) protoporphyrin IX to 4-methoxyacetophenone thiosemicarbazone via DFT-D3, MEP, QTAIM, NCI, ELF, and LOL studies. Journal of Molecular Modeling, 2017, 23, 200.	0.8	81
555	CO <sub>2</sub> Sequestration by Triazolylidene-Derived N-Heterocyclic Olefins: A Computational Study. ChemistrySelect, 2017, 2, 4648-4654.	0.7	9
556	Quantum chemical modeling of the reaction path of chorismate mutase based on the experimental substrate/product complex. FEBS Open Bio, 2017, 7, 789-797.	1.0	9
557	Intramolecularly Coordinated 2â€lminomethylphenyltellurium Compounds. European Journal of Inorganic Chemistry, 2017, 2017, 3435-3445.	1.0	5
558	Channeling through Two Stacked Guanine Quartets of One and Two Alkali Cations in the Li <sup>+</sup> , Na <sup>+</sup> , K <sup>+</sup> , and Rb <sup>+</sup> Series. Assessment of the Accuracy of the SIBFA Anisotropic Polarizable Molecular Mechanics Potential. Journal of Physical Chemistry B, 2017, 121, 3997-4014.	1.2	20
559	Molecular recognition of cyclodecapeptides to ibuprofen and naproxen enantiomers: a theoretical study. Structural Chemistry, 2017, 28, 1631-1644.	1.0	7
560	Side-by-Side Comparison of Hydroperoxide and Corresponding Alcohol as Hydrogen-Bond Donors. Journal of Physical Chemistry A, 2017, 121, 2951-2959.	1.1	29
561	A density functional theory study on the interactions between dibenzothiophene and tetrafluoroborate-based ionic liquids. Journal of Molecular Modeling, 2017, 23, 145.	0.8	12
562	Aromaticity of <i>peri</i> - and <i>para</i> -Substituted Naphthalene-1-carbaldehyde. Comparison with 1-Nitronaphthalene. Journal of Physical Chemistry A, 2017, 121, 2627-2635.	1.1	2
563	Microsolvation of the 5-hydroxyindole cation (5HI+) with nonpolar and quadrupolar ligands: Infrared photodissociation spectra of 5HI+-Ln clusters with L = Ar and N2 (n ≤3). Journal of Molecular Spectroscopy, 2017, 337, 124-136.	0.4	17
564	Perspective: Found in translation: Quantum chemical tools for grasping non-covalent interactions. Journal of Chemical Physics, 2017, 146, 120901.	1.2	90
565	Linear Ïfâ€Hole Bonding Dimers and Trimers Between Dihalogen Molecules XY (X, Y=Cl, Br) and Carbon Monoxide. ChemistrySelect, 2017, 2, 2687-2699.	0.7	9
566	GPU accelerated implementation of NCI calculations using promolecular density. Journal of Computational Chemistry, 2017, 38, 1071-1083.	1.5	7
567	The structure of Cu(II) and Hg(II) complexes of bispyrenyl azine revisited. Journal of Molecular Modeling, 2017, 23, 124.	0.8	0

#	Article	IF	CITATIONS
568	Theoretical insights into the π-hole interactions in the complexes containing triphosphorus hydride (P3H3) and its derivatives. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 195-202.	0.5	4
569	Taking the halogen bonding–hydrogen bonding competition one step further: complexes of difluoroiodomethane with trimethylphosphine, dimethyl sulfide and chloromethane. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 168-178.	0.5	12
570	Cinchona Alkaloid-Squaramide Catalyzed Sulfa-Michael Addition Reaction: Mode of Bifunctional Activation and Origin of Stereoinduction. Journal of Organic Chemistry, 2017, 82, 4362-4368.	1.7	57
571	Phosphazene Catalyzed Addition to Electron-Deficient Alkynes: The Importance of Nonlinear Allenyl Intermediates upon Stereoselectivity. Journal of Organic Chemistry, 2017, 82, 3855-3863.	1.7	24
572	Estimation of conventional C–Hâ<ï€ (arene), unconventional C–Hâ<ï€ (chelate) and C–Hâ<ï€ (thiocyanate) interactions in hetero-nuclear nickel( <scp>ii</scp> )–cadmium( <scp>ii</scp> ) complexes with a compartmental Schiff base. Dalton Transactions, 2017, 46, 5384-5397.	1.6	60
573	Synthesis and supramolecular self-assembly of thioxothiazolidinone derivatives driven by H-bonding and diverse π–hole interactions: A combined experimental and theoretical analysis. Journal of Molecular Structure, 2017, 1139, 209-221.	1.8	11
574	Catalytic Arene <i>meta</i> -C–H Functionalization Exploiting a Quinoline-Based Template. ACS Catalysis, 2017, 7, 3162-3168.	5.5	90
575	Computationally Designed 1,2,4-Triazolylidene-Derived N-Heterocyclic Olefins for CO <sub>2</sub> Capture, Activation, and Storage. ACS Omega, 2017, 2, 299-307.	1.6	16
576	Pursuit of Noncovalent Interactions for Strategic Site-Selective Catalysis. Accounts of Chemical Research, 2017, 50, 609-615.	7.6	188
577	Origin of Stereoselectivity in Cooperative Asymmetric Catalysis Involving N-Heterocyclic Carbenes and Lewis Acids toward the Synthesis of Spirooxindole Lactone. ACS Catalysis, 2017, 7, 530-537.	5.5	80
578	Mutations along a TET2 active site scaffold stall oxidation at 5-hydroxymethylcytosine. Nature Chemical Biology, 2017, 13, 181-187.	3.9	59
579	A Ligand-Dissociation-Involved Mechanism in Amide Formation of Monofluoroacylboronates with Hydroxylamines. Journal of Organic Chemistry, 2017, 82, 1064-1072.	1.7	13
580	Tuning Azoheteroarene Photoswitch Performance through Heteroaryl Design. Journal of the American Chemical Society, 2017, 139, 1261-1274.	6.6	244
581	Theoretical investigation of gas-phase molecular complex formation between 2-hydroxy thiophenol and a water molecule. Physical Chemistry Chemical Physics, 2017, 19, 2466-2478.	1.3	8
582	Design of van der Waals Two-Dimensional Heterostructures from Facially Polarized Janus All-Cis 1,2,3,4,5,6-Hexafluorocyclohexane (C6H6F6). Journal of Physical Chemistry C, 2017, 121, 1752-1762.	1.5	18
583	Thermal decomposition and biological activity of two supramolecular hybrid nitrates templated by piperazine. Journal of Thermal Analysis and Calorimetry, 2017, 127, 1553-1565.	2.0	4
584	Synthesis, crystal structure and DFT studies of a Zinc(II) complex of 1,3-diaminopropane (Dap), [Zn(Dap)(NCS)2][Zn(Dap)(NCS)2]n. The additional stabilizing role of Sâ<ï€ chalcogen bond. Journal of Molecular Structure, 2017, 1133, 271-277.	1.8	3
585	Toward more efficient densityâ€based adaptive QM/MM methods. International Journal of Quantum Chemistry, 2017, 117, e25336.	1.0	17

#	Article	IF	CITATIONS
586	Metal-free synthesis of quinolines catalyzed by carbon aerogels: Influence of the porous texture and surface chemistry. Chemical Engineering Journal, 2017, 314, 488-497.	6.6	25
587	Structural stability of diclofenac vs. inhibition activity from ab initio molecular dynamics simulations. Comparative study with ibuprofen and ketoprofen. Structural Chemistry, 2017, 28, 999-1008.	1.0	16
588	Asymmetric Biocatalytic Synthesis of Fluorinated Pyridines through Transesterification or Transamination: Computational Insights into the Reactivity of Transaminases. Advanced Synthesis and Catalysis, 2017, 359, 279-291.	2.1	20
589	Combined Utilization of <sup>1</sup> H NMR, IR, and Theoretical Calculations To Elucidate the Conformational Preferences of Some <scp>l</scp> -Histidine Derivatives. Journal of Physical Chemistry A, 2017, 121, 729-740.	1.1	9
590	Exploring Ultrashort Hydrogen–Hydrogen Nonbonded Contacts in Constrained Molecular Cavities. Journal of Physical Chemistry B, 2017, 121, 825-834.	1.2	23
591	Microsolvation of the pyrrole cation (Py <sup>+</sup> ) with nonpolar and polar ligands: infrared spectra of Py <sup>+</sup> –L <sub>n</sub> with L = Ar, N <sub>2</sub> , and H <sub>2</sub> O (n â‰\$). Physical Chemistry Chemical Physics, 2017, 19, 3970-3986.	1.3	36
592	A computational study of self-assembled hexapeptide inhibitors against amyloid-β (Aβ) aggregation. Physical Chemistry Chemical Physics, 2016, 19, 155-166.	1.3	18
593	Molecular Structure and Conformational Analysis of 1-Phenyl-1-X-1-Silacyclohexanes (X = F, Cl) by Electron Diffraction, Low-Temperature NMR, and Quantum Chemical Calculations. Journal of Organic Chemistry, 2017, 82, 461-470.	1.7	10
594	Mutation of Tyr137 of the universal <i>Escherichia coli</i> fimbrial adhesin FimH relaxes the tyrosine gate prior to mannose binding. IUCrJ, 2017, 4, 7-23.	1.0	19
595	Understanding a Hydroformylation Catalyst that Produces Branched Aldehydes from Alkyl Alkenes. Journal of the American Chemical Society, 2017, 139, 15921-15932.	6.6	63
596	Viable pathways for the oxidative addition of iodobenzene to palladium(0)-triphenylphosphine-carbonyl complexes: a theoretical study. Dalton Transactions, 2017, 46, 15789-15802.	1.6	12
597	Real-Space Bonding Indicator Analysis of the Donor–Acceptor Complexes X <sub>3</sub> BNY <sub>3</sub> , X <sub>3</sub> AlNY <sub>3</sub> , X <sub>, X<sub>3</sub>, X<sub>, X<sub>,</sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub></sub>	1.1	13
598	Exploiting the Ïfâ€Hole Concept: An Infrared and Ramanâ€Based Characterization of the Sâ‹â‹ô Chalcoge between 2,2,4,4â€Tetrafluoroâ€1,3â€dithiethane and Dimethyl Ether. Chemistry - A European Journal, 2017, 23, 17384-17392.		19
599	A DFT Study of N-Heterocyclic Carbene Catalyzed [4+2] Annulation between Saturated Carboxylate with <i>ortho</i> -Quinone Methide: Possible Mechanisms and Origin of Enantioselectivity. ChemistrySelect, 2017, 2, 8856-8864.	0.7	12
600	Role of Urea–Aromatic Stacking Interactions in Stabilizing the Aromatic Residues of the Protein in Urea-Induced Denatured State. Journal of the American Chemical Society, 2017, 139, 14931-14946.	6.6	47
601	Elucidation of Binding Site and Chiral Specificity of Oxidovanadium Drugs with Lysozyme through Theoretical Calculations. Inorganic Chemistry, 2017, 56, 12938-12951.	1.9	40
602	Nature and Strength of the Inner ore Hâ‹â‹A Interactions in Porphyrinoids. ChemPhysChem, 2017, 18, 3625-3633.	1.0	13
603	Mechanism and Origins of Stereoinduction in Natural Cinchona Alkaloid Catalyzed Asymmetric Electrophilic Trifluoromethylthiolation of Î <sup>2</sup> -Keto Esters with <i>N</i> -Trifluoromethylthiophthalimide as Electrophilic SCF <sub>3</sub> Source. ACS Catalysis, 2017 - 7077 7086	5.5	35

#	Article	IF	CITATIONS
604	DFT and AFIR Study on the Mechanism and the Origin of Enantioselectivity in Iron-Catalyzed Cross-Coupling Reactions. Journal of the American Chemical Society, 2017, 139, 16117-16125.	6.6	74
605	Exploring the origins of selectivity in soluble epoxide hydrolase from Bacillus megaterium. Organic and Biomolecular Chemistry, 2017, 15, 8827-8835.	1.5	14
606	Activation Mode and Origin of Selectivity in Chiral Phosphoric Acid-Catalyzed Oxacycle Formation by Intramolecular Oxetane Desymmetrizations. ACS Catalysis, 2017, 7, 7332-7339.	5.5	45
607	Asymmetric Induction in <i>C</i> -Alkylation of Tropane-Derived Enamines: Congruence Between Computation and Experiment. Journal of Organic Chemistry, 2017, 82, 10479-10488.	1.7	9
608	Following the Molecular Mechanism of Decarbonylation of Unsaturated Cyclic Ketones Using Bonding Evolution Theory Coupled with NCI Analysis. Journal of Physical Chemistry A, 2017, 121, 8504-8517.	1.1	40
609	Noncovalent interactions underlying binary mixtures of amino acid based ionic liquids: insights from theory. Physical Chemistry Chemical Physics, 2017, 19, 29561-29582.	1.3	1
610	Hybrid organic–inorganic CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> perovskite building blocks: Revealing ultraâ€strong hydrogen bonding and mulliken inner complexes and their implications in materials design. Journal of Computational Chemistry, 2017, 38, 2802-2818.	1.5	32
611	C–H···O Hydrogen Bonding. The Prototypical Methane-Formaldehyde System: A Critical Assessment. Journal of Chemical Theory and Computation, 2017, 13, 5379-5395.	2.3	17
612	Biological evaluation of dinuclear copper complex/dichloroacetic acid cocrystal against human breast cancer: design, synthesis, characterization, DFT studies and cytotoxicity assays. RSC Advances, 2017, 7, 47920-47932.	1.7	38
613	Two-Dimensional Arrangements of Bis(haloethynyl)benzenes Combining Halogen and Hydrogen Interactions. Crystal Growth and Design, 2017, 17, 6212-6223.	1.4	16
614	Statistics-Based Analysis of the Evolution of Structural and Electronic Properties of Realistic Amorphous Alumina During the Densification Process: Insights from First-Principles Approach. Journal of Physical Chemistry C, 2017, 121, 24745-24758.	1.5	4
615	Alkyl groups as electron density donors in π-hole bonding. CrystEngComm, 2017, 19, 6289-6296.	1.3	21
616	Ligand–Substrate Dispersion Facilitates the Copper-Catalyzed Hydroamination of Unactivated Olefins. Journal of the American Chemical Society, 2017, 139, 16548-16555.	6.6	189
617	Importance of Electrostatic Effects in the Stereoselectivity of NHC-Catalyzed Kinetic Resolutions. Journal of the American Chemical Society, 2017, 139, 12441-12449.	6.6	39
618	Attenuation of London Dispersion in Dichloromethane Solutions. Journal of the American Chemical Society, 2017, 139, 13126-13140.	6.6	93
619	Diradikaloid oder zwitterionischer Charakter: die ungesÃæigte Verbindung [Si <sub>4</sub> {N(SiMe <sub>3</sub> )Dipp} <sub>4</sub> ] mit gefaltetem Si <sub>4</sub> ‣trukturmotiv. Angewandte Chemie, 2017, 129, 14054-14059.	1.6	17
620	Diradicaloid or Zwitterionic Character: The Nonâ€īetrahedral Unsaturated Compound [Si <sub>4</sub> {N(SiMe <sub>3</sub> )Dipp} <sub>4</sub> ] with a Butterflyâ€type Si <sub>4</sub> Substructure. Angewandte Chemie - International Edition, 2017, 56, 13866-13871.	7.2	37
621	Origin of Stereoselectivity of the Photoinduced Asymmetric Phase-Transfer-Catalyzed Perfluoroalkylation of β-Ketoesters. Journal of Organic Chemistry, 2017, 82, 9321-9327.	1.7	36

#	Article	IF	CITATIONS
622	Solvent effect on the fixation of CO2 catalyzed by quaternary ammonium-based ionic liquids bearing different numbers of hydroxyl groups: A combined molecular dynamics simulation and ONIOM study. Molecular Catalysis, 2017, 441, 134-139.	1.0	15
623	All-metal aromatic cationic palladium triangles can mimic aromatic donor ligands with Lewis acidic cations. Chemical Science, 2017, 8, 7394-7402.	3.7	26
624	Binding of Thioflavin T and Related Probes to Polymorphic Models of Amyloid-β Fibrils. Journal of Physical Chemistry B, 2017, 121, 8926-8934.	1.2	34
625	Structural features of monohydrated 2-(4-fluorophenyl)ethylamine: a combined spectroscopic and computational study. Physical Chemistry Chemical Physics, 2017, 19, 23999-24008.	1.3	7
626	A topological study of chemical bonds under pressure: solid hydrogen as a model case. Physical Chemistry Chemical Physics, 2017, 19, 26381-26395.	1.3	7
627	Conformational landscape of isolated capped amino acids: on the nature of non-covalent interactions. European Physical Journal D, 2017, 71, 1.	0.6	3
628	Modulating the Proton Affinity of Silanol and Siloxane Derivatives by Tetrel Bonds. Journal of Physical Chemistry A, 2017, 121, 7424-7431.	1.1	16
629	The role of non-covalent interaction for the adsorption of CO <sub>2</sub> and hydrocarbons with per-hydroxylated pillar[6]arene: a computational study. New Journal of Chemistry, 2017, 41, 12044-12051.	1.4	32
630	Dialkylpyrazolium ionic liquids as novel catalyst for efficient fixation of CO2 with metal- and solvent-free. Applied Catalysis A: General, 2017, 547, 265-273.	2.2	37
631	A theoretical study of complexes between fullerenes and concave receptors with interest in photovoltaics. Physical Chemistry Chemical Physics, 2017, 19, 26787-26798.	1.3	25
632	DFT Investigation of Suzuki–Miyaura Reactions with Aryl Sulfamates Using a Dialkylbiarylphosphine-Ligated Palladium Catalyst. Organometallics, 2017, 36, 3664-3675.	1.1	15
633	Anthracenyl polar embedded stationary phases with enhanced aromatic selectivity. Part II: A density functional theory study. Journal of Chromatography A, 2017, 1519, 91-99.	1.8	2
634	The Role of Weak Interactions in Supramolecular Compounds: A Synthetic and Theoretical Study of Novel Elongated Cavitands. ChemistrySelect, 2017, 2, 8337-8345.	0.7	5
635	Frustrated Lewis Trios and Longâ€Range Hole Interactions: A Combined Structural and Theoretical Study of LBâ^'AX <sub>3</sub> â‹â‹â‹â‹LB and LBâ‹â‹â‹AX <sub>3</sub> â‹â‹â‹LB (A=B, Al, Ga, In) 18, 2864-2872.	Sys <b>teo</b> ns. C	Che <b>no</b> PhysChe
636	Structural effects of trifluoromethylation and fluorination in gold( <scp>i</scp> ) BIPHEP fluorothiolates. New Journal of Chemistry, 2017, 41, 10537-10541.	1.4	7
637	Theoretical investigation of the π + -π + stacking interactions in substituted pyridinium ion. Journal of Molecular Graphics and Modelling, 2017, 77, 225-231.	1.3	7
638	Is the R <sub>3</sub> Si Moiety in Metal–Silyl Complexes a Z ligand? An Answer from the Interaction Energy. Chemistry - A European Journal, 2017, 23, 17058-17069.	1.7	25
639	A molecular electron density theory study of [3Â+Â2] cycloaddition reactions of chiral azomethine ylides with β-nitrostyrene. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	21

#	Article	IF	CITATIONS
640	Computational Simulations of DNA Polymerases: Detailed Insights on Structure/Function/Mechanism from Native Proteins to Cancer Variants. Chemical Research in Toxicology, 2017, 30, 1922-1935.	1.7	19
641	Dimethyl Sulfoxide Complexes Detected at Ambient Conditions. Journal of Physical Chemistry A, 2017, 121, 6046-6053.	1.1	6
642	Quantitative probing of subtle interactions among H-bonds in alpha hydroxy carboxylic acid complexes. Physical Chemistry Chemical Physics, 2017, 19, 24399-24411.	1.3	6
643	Theoretical study on the cage-like nanostructures formed by amino acids andÂtheir potential applications as drug carriers. Molecular Physics, 2017, 115, 3051-3066.	0.8	0
644	Theoretical investigation of hydrogen bonding in the H 2 SO 4 â⊄HNO 3 system. Computational and Theoretical Chemistry, 2017, 1117, 41-46.	1.1	6
645	Theoretical study on selectivity trends in ( <i>N</i> â€heterocyclic carbene)â€Pd catalyzed mizoroki–heck reactions: Exploring density functionals methods and molecular models. Journal of Computational Chemistry, 2017, 38, 2371-2377.	1.5	13
646	Conformational preferences of protonated N-acetylated hexosamines probed by InfraRed Multiple Photon Dissociation (IRMPD) spectroscopy and ab initio calculations. International Journal of Mass Spectrometry, 2017, 421, 116-123.	0.7	27
647	Artificial Chiral Metallo-pockets Including a Single Metal Serving as Structural Probe and Catalytic Center. CheM, 2017, 3, 174-191.	5.8	62
648	Interaction between anti-cancer drug hydroxycarbamide and boron nitride nanotube: A long-range corrected DFT study. Computational and Theoretical Chemistry, 2017, 1117, 61-80.	1.1	19
649	Novel electrochemical route to cleaner fuel dimethyl ether. Scientific Reports, 2017, 7, 6901.	1.6	22
650	Linear σ-holeâ√C Oâ√σ-hole intermolecular interactions between carbon monoxide and dihalogen molecules XY (X, Y = Cl, Br). Journal of Molecular Graphics and Modelling, 2017, 76, 419-428.	1.3	6
651	Bonding in Heavier Group 14 Zeroâ€Valent Complexes—A Combined Maximum Probability Domain and Valence Bond Theory Approach. Chemistry - A European Journal, 2017, 23, 14604-14613.	1.7	14
652	Mechanism of Amide Bond Formation from Carboxylic Acids and Amines Promoted by 9-Silafluorenyl Dichloride Derivatives. Journal of Organic Chemistry, 2017, 82, 9087-9096.	1.7	18
653	A Simple Isomerization of the Purine Scaffold of a Kinase Inhibitor, Roscovitine, Affords a Four- to Seven-Fold Enhancement of Its Affinity for Four CDKs. Could This Be Traced Back to Conjugation-Induced Stiffenings/Loosenings of Rotational Barriers?. ACS Omega, 2017, 2, 3467-3474.	1.6	8
654	Change in optoelectronic properties of ExBox <sup>+4</sup> on functionalization and guest encapsulation. Physical Chemistry Chemical Physics, 2017, 19, 23373-23385.	1.3	10
655	Unravelling hydrogen bonding interactions of tryptamine–water dimer from neutral to cation. Physical Chemistry Chemical Physics, 2017, 19, 25260-25269.	1.3	6
656	Endohedral gas adsorption by cucurbit[7]uril: a theoretical study. Physical Chemistry Chemical Physics, 2017, 19, 24448-24452.	1.3	13
657	How the electron-deficient cavity of heterocalixarenes recognizes anions: insights from computation. Physical Chemistry Chemical Physics, 2017, 19, 24696-24705.	1.3	29

	CITATION R	DN REPORT		
#	Article	IF	CITATIONS	
658	Calix[4]arene-fused phospholes. Dalton Transactions, 2017, 46, 9833-9845.	1.6	19	
659	Non-covalent green functionalization of boron nitride nanotubes with tunable aryl alkyl ionic liquids: A quantum chemical approach. Journal of Molecular Liquids, 2017, 243, 22-40.	2.3	13	
660	The silane–methane dimer revisited: more than a dispersion-bound system?. Physical Chemistry Chemical Physics, 2017, 19, 32663-32669.	1.3	11	
661	Intramolecular Siâ‹â‹â‹O Tetrel Bonding: Tuning of Substituents and Cooperativity. ChemistrySelect, 2017 11104-11112.	, 2, <sub>0.7</sub>	8	
662	The π–π stacking of tanshinone I and isotanshinone I with phenylalanine: The effects of isomerization, complexation and environment. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750067.	1.8	1	
663	Electronic structure and bonding of the dinuclear metal M2(CO)10 decacarbonyls: applications of natural orbitals for chemical valence. Journal of Molecular Modeling, 2017, 23, 358.	0.8	2	
664	Heterolytic Splitting of Molecular Hydrogen by Frustrated and Classical Lewis Pairs: A Unified Reactivity Concept. Scientific Reports, 2017, 7, 16024.	1.6	40	
665	QM/MM Study of the Reaction Catalyzed by Alkyladenine DNA Glycosylase: Examination of the Substrate Specificity of a DNA Repair Enzyme. Journal of Physical Chemistry B, 2017, 121, 11096-11108.	1.2	14	
666	Unveiling Mechanism of a Quinine-Squaramide Catalyzed Enantioselective Aza-Friedel–Crafts Reaction between Cyclic Trifluoromethyl Ketimine and Naphthol: A DFT Study. Journal of Organic Chemistry, 2017, 82, 13109-13114.	1.7	10	
667	Non-covalent interactions in the multicomponent crystal of 1-aminocyclopentane carboxylic acid, oxalic acid and water: a crystallographic and a theoretical approach. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 968-980.	0.5	10	
668	Comparing Structure and Dynamics of Solvation of Different Iron Oxide Phases for Enhanced Magnetic Resonance Imaging. ChemistrySelect, 2017, 2, 10136-10142.	0.7	13	
669	Supramolecular Design of the Trinuclear Silver(I) and Copper(I) Metal Pyrazolates Complexes with Ruthenium Sandwich Compounds via Intermolecular Metalâ^'i€ Interactions. Crystal Growth and Design, 2017, 17, 6770-6779.	1.4	28	
670	Reactivity and regioselectivity in Diels–Alder reactions of anion encapsulated fullerenes. Physical Chemistry Chemical Physics, 2017, 19, 30393-30401.	1.3	19	
671	Metal-porphyrin catalyzed aziridination of α-methylstyrene: Batch vs. flow process. Journal of Porphyrins and Phthalocyanines, 2017, 21, 381-390.	0.4	6	
672	Importance of R–CF <sub>3</sub> ···O Tetrel Bonding Interactions in Biological Systems. Journal of Physical Chemistry A, 2017, 121, 5371-5376.	1.1	69	
673	Weak hydrogen bonds in adsorption of nonrigid molecules on graphitized thermal carbon black. Journal of Structural Chemistry, 2017, 58, 558-584.	0.3	3	
674	Conformational flexibility and base-pairing tendency of the tobacco carcinogen O6-[4-oxo-4-(3-pyridyl)butyl]guanine. Biophysical Chemistry, 2017, 228, 25-37.	1.5	5	
675	Intramolecular C Sâ< <sup>-</sup> O S(C) chalcogen bonds: A theoretical study of the effects of substituents and intermolecular hydrogen bonds. Computational and Theoretical Chemistry, 2017, 1115, 190-196.	1.1	8	

#	Article	IF	CITATIONS
676	Experimental and theoretical distribution of electron density and thermopolimerization in crystals of Ph 3 Sb(O 2 CCH=CH 2 ) 2 complex. Journal of Solid State Chemistry, 2017, 254, 32-39.	1.4	11
677	Crystal Structure of the DFNKF Segment of Human Calcitonin Unveils Aromatic Interactions between Phenylalanines. Chemistry - A European Journal, 2017, 23, 2051-2058.	1.7	28
678	On the origin of the relative stability of Zn <sup>II</sup> NTA and Zn <sup>II</sup> NTPA metal complexes. An insight from the IQA, IQF, and I€â€FARMS methods. International Journal of Quantum Chemistry, 2017, 117, e25321.	1.0	5
679	Characterization of non-classical C Brâ∢ï€ interactions in (E)-1,3-dibromo-5-(2-(ferrocenyl)vinyl)benzene and related derivatives of ferrocene. Journal of Molecular Structure, 2017, 1131, 16-24.	1.8	7
680	Sizing the role of London dispersion in the dissociation of all-meta tert-butyl hexaphenylethane. Chemical Science, 2017, 8, 405-410.	3.7	104
681	A DFT study of the mechanism and selectivities of the [3Â+Â2] cycloaddition reaction between 3â€{benzylideneamino)oxindole and <i>trans</i> â€Î²â€nitrostyrene. Journal of Physical Organic Chemistry, 2017, 30, e3637.	0.9	22
682	pH controlled assembly of a self-complementary halogen-bonded dimer. Chemical Science, 2017, 8, 938-945.	3.7	23
683	Exploration of photocatalytic activity of an end-on azide bridged one-dimensional cadmium(II) Schiff base complex for the degradation of organic dye in visible light. Polyhedron, 2017, 121, 199-205.	1.0	26
684	Investigating carbohydrate based ligands for galectin-3 with docking and molecular dynamics studies. Journal of Molecular Graphics and Modelling, 2017, 71, 211-217.	1.3	5
685	Visualization of Biomolecular Structures: State of the Art Revisited. Computer Graphics Forum, 2017, 36, 178-204.	1.8	69
686	Experimental observation of charge-shift bond in fluorite CaF <sub>2</sub> . Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 643-653.	0.5	8
687	Topological Data Analysis for Scientific Visualization. Mathematics and Visualization, 2017, , .	0.4	16
688	3. Qualitative and quantitative crystal engineering of multi-functional co-crystals. , 2017, , 60-102.		1
689	Conformational study of L-methionine and L-cysteine derivatives through quantum chemical calculations and 3 J HH coupling constant analyses. Beilstein Journal of Organic Chemistry, 2017, 13, 925-937.	1.3	5
690	Progress in the Understanding of Traditional and Nontraditional Molecular Interactions. , 2017, , 67-100.		4
691	Solving the scalability issue in quantum-based refinement: Q R#1. Acta Crystallographica Section D: Structural Biology, 2017, 73, 1020-1028.	1.1	20
692	Hapticity of asymmetric rhodium-allyl compounds in the light of real-space bonding indicators. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 615-626.	0.4	0
693	The physicochemical properties and tyrosinase inhibitory activity of ectoine and its analogues: A theoretical study. Computational and Theoretical Chemistry, 2018, 1130, 6-14.	1.1	5

#	Article	IF	CITATIONS
694	Kinetic and mechanistic insight into the formation of amphetamine using the Leuckart–Wallach reaction and interaction of the drug with GpC·CpG base-pair step of DNA: a DFT study. Monatshefte Für Chemie, 2018, 149, 1045-1057.	0.9	6
695	Interactions of Schiff base compounds and their coordination complexes with the drug cisplatin. New Journal of Chemistry, 2018, 42, 5834-5843.	1.4	22
696	Mechanistic insights into asymmetric reductive coupling of isoquinolines by a chiral diboron with DFT calculations. Journal of Organometallic Chemistry, 2018, 864, 97-104.	0.8	13
697	DFT calculations and NMR measurements applied to the conformational analysis of cis and trans -3-phenylaminocyclohexyl N,N -dimethylcarbamates. Journal of Molecular Structure, 2018, 1163, 227-235.	1.8	3
698	Solvation of diclofenac in water from atomistic molecular dynamics simulations – interplay between solute–solute and solute–solvent interactions. Physical Chemistry Chemical Physics, 2018, 20, 8629-8639.	1.3	18
699	A molecular electron density theory study of the [3Â+Â2] cycloaddition reaction between an azomethine imine and electron deficient ethylenes. Journal of Physical Organic Chemistry, 2018, 31, e3830.	0.9	22
700	Recognition of Melamine by Chromium Tricarbonyl (Thio)barbituric Acid Derivatives: Theoretical Insight into Multiple Hydrogenâ€Bond Modes. ChemistrySelect, 2018, 3, 2404-2415.	0.7	0
701	Site specificity of halogen bonding involving aromatic acceptors. Physical Chemistry Chemical Physics, 2018, 20, 8685-8694.	1.3	19
702	Anisotropic lattice softening near the structural phase transition in the thermosalient crystal 1,2,4,5-tetrabromobenzene. Physical Chemistry Chemical Physics, 2018, 20, 8523-8532.	1.3	31
703	Enantiocontrol by assembled attractive interactions in copper-catalyzed asymmetric direct alkynylation of α-ketoesters with terminal alkynes: OH⋯O/sp <sup>3</sup> -CH⋯O two-point hydrogen bonding combined with dispersive attractions. Chemical Science, 2018, 9, 3484-3493.	3.7	43
704	Revealing the Conformational Preferences of Proteinogenic Glutamic Acid Derivatives in Solution by <sup>1</sup> H NMR Spectroscopy and Theoretical Calculations. Journal of Physical Chemistry A, 2018, 122, 4555-4561.	1.1	2
705	Weak Intermolecular Interactions. , 2018, , 289-319.		3
706	Schwere Carbenhomologe: donorfreie Bismutenium―und Stibeniumâ€ŧonen. Angewandte Chemie, 2018, 130, 10237-10241.	1.6	30
707	Survey of short and long cuprophilic d <sup>10</sup> –d <sup>10</sup> contacts for tetranuclear copper clusters. Understanding of bonding and ligand role from a planar superatom perspective. New Journal of Chemistry, 2018, 42, 8874-8881.	1.4	5
708	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. Chemistry - A European Journal, 2018, 24, 9853-9859.	1.7	28
709	Quest for Insight into Ultrashort C–H··Ĩ€ Proximities in Molecular "Iron Maidens― Journal of Organic Chemistry, 2018, 83, 5114-5122.	1.7	8
710	Sulfur(lone-pair)…π interactions with FAD in flavoenzymes. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 531-537.	0.4	6
711	Yoink: An interactionâ€based partitioning API. Journal of Computational Chemistry, 2018, 39, 799-806.	1.5	13

ARTICLE IF CITATIONS Fullerene size controls the selective complexation of [11]CPP with pristine and endohedral 712 1.3 26 fullerenes. Physical Chemistry Chemical Physics, 2018, 20, 11347-11358. Computational Screening of New Orthogonal Metalâ€Free Dipolar Cycloadditions of Mesomeric 1.7 Betaines. Chemistry - A European Journal, 2018, 24, 7507-7512. Heavy Carbene Analogues: Donorâ€Free Bismuthenium and Stibenium Ions. Angewandte Chemie -714 7.2 55 International Edition, 2018, 57, 10080-10084. Influence of substituents and cooperativity in doubly hydrogen-bonded complexes of 2-pyridone and 0.8 oxalic acid. Molecular Physics, 2018, 116, 1862-1870. Influence of different substitution in pyrazolium ionic liquids on catalytic activity for the fixation of 716 1.0 15 CO2 under solvent- and metal-free conditions. Tetrahedron, 2018, 74, 1776-1784. The ability of Ex<sup>2</sup>Box<sup>4+</sup> to interact with guests containing πâ€electronâ€rich and 1.0 Ï€â€electronâ€poor moieties. International Journal of Quantum Chemistry, 2018, 1Ĭ8, e25607. Understanding the molecular mechanism of thio-Claisen rearrangement of allyl phenyl sulfide and allyl vinyl sulfide using bonding evolution theory coupled with NČI analysis. Journal of Sulfur Chemistry, 2018, 39, 350-366. 718 1.0 10 Rhodium Catalyzed Asymmetric Hydroamination of Internal Alkynes with Indoline: Mechanism, Origin 1.7 of Enantioselectivity, and Role of Ádditives. Journal of Organic Chemistry, 2018, 83, 2627-2639. Computational Unravelling of the Role of Alkyl Groups on the Hostâ€Guest Complexation of 720 0.7 18 Pillar[5]arenes with Neutral Dihalobutanes. ChemistrySelect, 2018, 3, 1321-1334. Supramolecular polymer chemistry meets computational chemistry: theoretical simulations on 1.5 advanced self-assembling chiral materials. Supramolecular Chemistry, 2018, 30, 876-890. Organocatalyzed Asymmetric Vinylogous Addition of Oxazole- $2(3\langle i\rangle H \langle i \rangle)$ -thiones to  $\hat{I}_{\pm}, \hat{I}^2$ -Unsaturated Ketones: An Additive-Free Approach for Diversification of Heterocyclic Scaffold. Journal of Organic 722 7 1.7 Chemistry, 2018, 83, 1701-1716. Reconsideration of the Detection and Fluorescence Mechanism of a Pyrene-Based Chemosensor for 1.1 TNT. Journal of Physical Chemistry A, 2018, 122, 1400-1405. Hydrogen-Bonding Acceptor Character of Be<sub>3</sub>, the Beryllium Three-Membered Ring. 724 1.1 15 Journal of Physical Chemistry A, 2018, 122, 1472-1478. A theoretical study on the mechanism of hydrogenation of carboxylic acids catalyzed by the Saito catalyst. Dalton Transactions, 2018, 47, 2460-2469. 1.6 Ab initio calculations, structure, NBO and NCI analyses of X Hâ√i€ interactions. Chemical Physics Letters, 726 1.2 15 2018, 693, 202-209. Large-Scale Functional Group Symmetry-Adapted Perturbation Theory on Graphical Processing Units. Journal of Chemical Theory and Computation, 2018, 14, 1737-1753. Application of the Interacting Quantum Atoms Approach to the S66 and Ionicâ€Hydrogenâ€Bond Datasets 728 1.0 21 for Noncovalent Interactions. ChemPhysChem, 2018, 19, 973-987. Microhydration of PAH<sup>+</sup> cations: evolution of hydration network in naphthalene<sup>+</sup>-(H<sub>2</sub>O)<sub>n</sub> clusters (<i>n</i>) â‰5). Chemical Science, 729 2018, 9, 2301-2318.

#	ARTICLE	IF	CITATIONS
730	On the σ, π and δ hole interactions: a molecular orbital overview. New Journal of Chemistry, 2018, 42, 1413-1422.	1.4	72
731	Characterization of the one-electron oxidized Cu(II)-salen complexes with a side chain aromatic ring: the effect of the indole ring on the Cu(II)-phenoxyl radical species. Journal of Biological Inorganic Chemistry, 2018, 23, 51-59.	1.1	16
732	A detailed hydrogen bonding analysis on the compositions of H 2 SO 4 /HNO 3 /H 2 O ternary systems: A computational study. Journal of Molecular Graphics and Modelling, 2018, 80, 272-281.	1.3	2
733	Hydrogen-bonding behavior of various conformations of the HNO3… (CH3OH)2 ternary system. Journal of Molecular Modeling, 2018, 24, 23.	0.8	1
734	The Independent Gradient Model: A New Approach for Probing Strong and Weak Interactions in Molecules from Wave Function Calculations. ChemPhysChem, 2018, 19, 724-735.	1.0	263
735	Protic pyrazolium ionic liquids for efficient chemical fixation of CO <sub>2</sub> : design, synthesis, and catalysis. Molecular Systems Design and Engineering, 2018, 3, 348-356.	1.7	16
736	Control of Chain Walking by Weak Neighboring Group Interactions in Unsymmetrical Catalysts. Journal of the American Chemical Society, 2018, 140, 1305-1312.	6.6	80
737	Bending Carbon Nanoforms for Supramolecular Recognition: A Topological Study on Hemifullerene-Based Aggregates. Journal of Physical Chemistry A, 2018, 122, 1124-1137.	1.1	5
738	V <sup>IV</sup> O complexes with antibacterial quinolone ligands and their interaction with serum proteins. Dalton Transactions, 2018, 47, 2164-2182.	1.6	36
739	Enantioselective Vinylogous Amination of 5-Alkyl-4-nitroisoxazoles with a Dipeptide-Based Guanidinium Phase-Transfer Catalyst. Organic Letters, 2018, 20, 429-432.	2.4	36
740	Novel Brâ‹â‹ï€(Chelate) Interaction in a 1D Coordination Polymer Revealing Aromaticity. ChemistrySelect, 2018, 3, 4289-4291.	0.7	18
741	Protic Quaternary Ammonium Ionic Liquids for Catalytic Conversion of CO <sub>2</sub> into Cyclic Carbonates: A Combined Ab Initio and MD Study. Industrial & Engineering Chemistry Research, 2018, 57, 7121-7129.	1.8	14
742	Evolution of molecular packing and rheology in asphalt binder during rejuvenation. Fuel, 2018, 222, 457-464.	3.4	55
743	Drastic Stabilization of Junction Nodes in Supramolecular Structures Based on Host–Guest Complexes. Macromolecules, 2018, 51, 2732-2741.	2.2	21
744	DFT study of nanotubes as the drug delivery vehicles of Efavirenz. Computational and Theoretical Chemistry, 2018, 1131, 57-68.	1.1	42
745	Towards a better understanding of the parameters determining the competition between bromine halogen bonding and hydrogen bonding: An FTIR spectroscopic study of the complexes between bromodifluoromethane and trimethylamine. Journal of Molecular Structure, 2018, 1165, 349-355.	1.8	8
746	Catching TFSI: A Computational–Experimental Approach to β yclodextrinâ€Based Host–Guest Systems as electrolytes for Liâ€Ion Batteries. ChemSusChem, 2018, 11, 1942-1949.	3.6	3
747	The effect of benzoâ€annelation on intermolecular hydrogen bond and proton transfer of 2â€methylâ€3â€hydroxyâ€4( <scp><i>1H</i></scp> )â€quinolone in methanol: A <scp>TDâ€DFT</scp> study. Jou Physical Organic Chemistry, 2018, 31, e3803.	rma9of	5

#	Article	IF	CITATIONS
748	Effect of pH on Eosin Y/PAMAM interactions studied from absorption spectroscopy and molecular dynamics simulations. Journal of Luminescence, 2018, 199, 258-265.	1.5	11
749	Hybridization of Nitrogen Determines Hydrogen-Bond Acceptor Strength: Gas-Phase Comparison of Redshifts and Equilibrium Constants. Journal of Physical Chemistry A, 2018, 122, 3899-3908.	1.1	8
750	Catalytic mechanism and molecular engineering of quinolone biosynthesis in dioxygenase AsqJ. Nature Communications, 2018, 9, 1168.	5.8	30
751	1,8-Bis(diphenylphosphino)biphenylene. A new ligand for late transition metal complexes. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 627-639.	0.4	7
752	Non-covalent interaction in benzene and substituted benzene: A theoretical study. Computational and Theoretical Chemistry, 2018, 1130, 134-139.	1.1	29
753	Intermolecular interactions between σ- and π-holes of bromopentafluorobenzene and pyridine: computational and experimental investigations. Physical Chemistry Chemical Physics, 2018, 20, 11386-11395.	1.3	15
754	Theoretical insight into phosphoric acid-catalyzed asymmetric conjugate addition of indolizines to α,β-unsaturated ketones. Chinese Chemical Letters, 2018, 29, 1237-1241.	4.8	26
755	Understanding the Origin of Phosphorescence in Bismoles: A Synthetic and Computational Study. Inorganic Chemistry, 2018, 57, 7536-7549.	1.9	34
756	Abnormal Tetrel Bonds between Formamidine and TH <sub>3</sub> F: Substituent Effects. ChemistrySelect, 2018, 3, 2842-2849.	0.7	9
757	Functionalized carbon black nanoparticles used for separation of emulsified oil from oily wastewater. Journal of Dispersion Science and Technology, 2018, 39, 497-506.	1.3	30
758	Role of 6-Mercaptopurine in the potential therapeutic targets DNA base pairs and G-quadruplex DNA: insights from quantum chemical and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2018, 36, 1369-1401.	2.0	16
759	Protonation of methyluracils in the gas phase: The particular case of 3-methyluracil. International Journal of Mass Spectrometry, 2018, 429, 47-55.	0.7	9
760	Sequential microhydration of cationic 5-hydroxyindole (5HI <sup>+</sup> ): infrared photodissociation spectra of 5HI <sup>+</sup> –W <sub>n</sub> clusters (W = H <sub>2</sub> O,) Tj ETQq0 0	01r.gBT /O	vezłack 10 T
761	Penta and hexacoordinated aluminum(III) compounds containing benzotriazole and benzimidazole derivatives as ligands. Inorganica Chimica Acta, 2018, 471, 1-7.	1.2	1
762	Dissecting the concave–convex Ï€â€₩ interaction in corannulene and sumanene dimers: SAPT(DFT) analysis and performance of DFT dispersionâ€corrected methods. Journal of Computational Chemistry, 2018, 39, 93-104.	1.5	12
763	Synthesis, structure, computational and in-silico anticancer studies of N,N -diethyl- N ′-palmitoylthiourea. Journal of Molecular Structure, 2018, 1153, 69-77.	1.8	20
764	Densityâ€functional theory study of the interaction mechanism and optical properties of flavonols on the boron nitride nanotubes. International Journal of Quantum Chemistry, 2018, 118, e25514.	1.0	12
765	Synthesis and halogenation of bis(8-methoxynaphthyl)ditelluride. Inorganica Chimica Acta, 2018, 475, 73-82.	1.2	4

#	Article	IF	CITATIONS
766	Host–guest interactions between octa acid and cations/nucleobases. Journal of Computational Chemistry, 2018, 39, 161-175.	1.5	12
767	The crystal structures of 1-(4-halo-2,3,5,6-tetrafluorophenyl)-3-benzylimidazolium bromides: The relative importance of anion–Ĩ€, lone pair–Ĩ€, Ï€ Ï€ stacking and halogen bonding interactions. Journal of Fluorine Chemistry, 2018, 206, 61-71.	0.9	13
768	Single X-ray crystal structure, DFT studies and topoisomerase I inhibition activity of a tailored ionic Ag( <scp>i</scp> ) nalidixic acid–piperazinium drug entity specific for pancreatic cancer cells. New Journal of Chemistry, 2018, 42, 506-519.	1.4	20
769	A possible reason behind the initial formation of pentagonal dodecahedron cavities in sI-methane hydrate nucleation: A DFT study. Chemical Physics Letters, 2018, 691, 415-420.	1.2	3
770	Confinement induced thermodynamic and kinetic facilitation of some Diels–Alder reactions inside a CB[7] cavitand. Journal of Computational Chemistry, 2018, 39, 151-160.	1.5	34
771	Ion-pair recognition based on halogen bonding: a case of the crown-ether receptor with iodo-trizole moiety. Structural Chemistry, 2018, 29, 533-540.	1.0	7
772	Large Protonâ€Affinity Enhancements Triggered by Noncovalent Interactions. Chemistry - A European Journal, 2018, 24, 1971-1977.	1.7	15
773	Quantum chemical analysis of electronic structure and bonding aspects of choline based ionic liquids. Journal of Molecular Liquids, 2018, 249, 637-649.	2.3	19
774	Revisiting the racemization mechanism of helicenes. Chemical Communications, 2018, 54, 188-191.	2.2	107
775	Characterization of chalcogen bonding interactions via an inâ€depth conceptual quantum chemical analysis. Journal of Computational Chemistry, 2018, 39, 557-572.	1.5	53
776	Investigation of carboxylation of carbon nanotube in the adsorption of anti-cancer drug: A theoretical approach. Applied Surface Science, 2018, 427, 112-125.	3.1	21
777	Solvomorphs of tyraminium 5,5-diethylbarbiturate: a rare example of the barbiturate <i>R</i> <sub>3</sub> <sup>3</sup> (12) hydrogen-bond motif and a crystal structure with <i>Z</i> ′ = 4. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 1586-1594.	0.2	1
778	Controlling the Functional Properties of Oligothiophene Crystalline Nano/Microfibers via Tailoring of the Selfâ€Assembling Molecular Precursors. Advanced Functional Materials, 2018, 28, 1801946.	7.8	21
779	The Importance of CH···X (X = O, π) Interaction of a New Mixed Ligand Cu(II) Coordination Polymer: Structure, Hirshfeld Surface and Theoretical Studies. Crystals, 2018, 8, 455.	1.0	47
780	Probing chirality recognition of protonated glutamic acid dimers by gas-phase vibrational spectroscopy and first-principles simulations. Physical Chemistry Chemical Physics, 2018, 20, 28452-28464.	1.3	19
781	Infrared spectroscopy of gas phase alpha hydroxy carboxylic acid homo and hetero dimers. Physical Chemistry Chemical Physics, 2018, 20, 29601-29609.	1.3	1
782	Assessment of electronic transitions involving intermolecular charge transfer in complexes formed by fullerenes and donor–acceptor nanohoops. Physical Chemistry Chemical Physics, 2018, 20, 27791-27803.	1.3	5
783	The role played by ethanol in achieving the successive <i>versus</i> simultaneous mechanism of excited-state double proton transfer in dipyrido[2,3- <i>a</i> :3′,2′- <i>i</i> ]carbazole. Physical Chemistry Chemical Physics, 2018, 20, 26259-26265.	1.3	47

#	Article	IF	CITATIONS
784	Nature of cucurbituril–halogen encapsulation. Structural and interaction energy consideration in the X <sub>2</sub> @CB[ <i>n</i> ] (X = Cl, Br, l, <i>n</i> = 6, 7, 8) from relativistic DFT calculations. Physical Chemistry Chemical Physics, 2018, 20, 29325-29332.	1.3	7
785	Computational investigations of intermolecular interactions between electron-accepting bromo- and iodo-pentafluorobenzene and electron-donating furan and thiophene. New Journal of Chemistry, 2018, 42, 20101-20112.	1.4	5
786	Theoretical study of ethanol interaction with pristine and P-doped single-walled carbon nanotubes. Materials Today: Proceedings, 2018, 5, 11043-11050.	0.9	0
787	Intramolecular P–H··Ĥ–Si Dihydrogen Bonding in the 5-Dimethylsilyl-9,9-dimethylxanthen-4-yl-diphenylphosphonium Cation. Organometallics, 2018, 37, 4287-4296.	1.1	4
788	Chemical bonding origin of the unexpected isotropic physical properties in thermoelectric Mg3Sb2 andÂrelated materials. Nature Communications, 2018, 9, 4716.	5.8	102
789	Weak interactions in furan dimers. Journal of Computer-Aided Molecular Design, 2018, 32, 1247-1258.	1.3	5
790	Direct Asymmetric Hydrogenation of <i>N</i> -Methyl and <i>N</i> -Alkyl Imines with an Ir(III)H Catalyst. Journal of the American Chemical Society, 2018, 140, 16967-16970.	6.6	47
791	Switching of binding site from nonpolar to polar ligands toward cationic benzonitrile revealed by infrared spectroscopy. Journal of Chemical Physics, 2018, 149, 174315.	1.2	14
792	Quantitative Assessment of Tetrel Bonding Utilizing Vibrational Spectroscopy. Molecules, 2018, 23, 2763.	1.7	84
793	Polarizable ab initio QM/MM Study of the Reaction Mechanism of N-tert-Butyloxycarbonylation of Aniline in [EMIm][BF4]. Molecules, 2018, 23, 2830.	1.7	10
794	Characterizing Molecular Adsorption on Biodegradable MnO <sub>2</sub> Nanoscaffolds. Journal of Physical Chemistry C, 2018, 122, 29017-29027.	1.5	11
795	Isomerism of the Aniline Trimer. Angewandte Chemie, 2018, 130, 15332-15336.	1.6	6
796	Analysis of two [2]catenanes based on electron densities from invariom refinement and results from DFT calculations. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2018, 73, 677-687.	0.3	3
797	Sâ‹â‹â‹Sn Tetrel Bonds in the Activation of Peroxisome Proliferatorâ€Activated Receptors (PPARs) by Organotin Molecules. Chemistry - A European Journal, 2018, 24, 16582-16587.	1.7	35
798	Comparing quantitative prediction methods for the discovery of small-molecule chiral catalysts. Nature Reviews Chemistry, 2018, 2, 290-305.	13.8	100
799	Isomerism of the Aniline Trimer. Angewandte Chemie - International Edition, 2018, 57, 15112-15116.	7.2	19
800	Probing the Delicate Balance between Pauli Repulsion and London Dispersion with Triphenylmethyl Derivatives. Journal of the American Chemical Society, 2018, 140, 14421-14432.	6.6	70
801	Building Fluorinated Hybrid Crystals: Understanding the Role of Noncovalent Interactions. Crystal Growth and Design, 2018, 18, 6901-6910.	1.4	14

#	Article	IF	CITATIONS
802	Insight on <i>asym</i> -Pyrazolium Ionic Liquids for Chemical Fixation of CO <sub>2</sub> and Propylene Epoxide into Propylene Carbonate without Organic Solvent and Metal. Industrial & Engineering Chemistry Research, 2018, 57, 13342-13352.	1.8	10
803	A Computational Study on the 4â€Dimethylaminopyridine (DMAP)â€Catalyzed Regioselective [2+4] Cyclization of Allenic Ester with Cyclic Ketimine. ChemistrySelect, 2018, 3, 10553-10558.	0.7	7
804	The adsorption of bromomethane onto the exterior surface of aluminum nitride, boron nitride, carbon, and silicon carbide nanotubes: A PBC-DFT, NBO, and QTAIM study. Computational and Theoretical Chemistry, 2018, 1144, 26-37.	1.1	56
805	The Nonlocal Kernel in van der Waals Density Functionals as an Additive Correction: An Extensive Analysis with Special Emphasis on the B97M-V and ωB97M-V Approaches. Journal of Chemical Theory and Computation, 2018, 14, 5725-5738.	2.3	170
806	Probing the Influence of PAd-DalPhos Ancillary Ligand Structure on Nickel-Catalyzed Ammonia Cross-Coupling. Organometallics, 2018, 37, 4015-4023.	1.1	10
807	Modulation of Ïf-Alkane Interactions in [Rh(L <sub>2</sub> )(alkane)] <sup>+</sup> Solid-State Molecular Organometallic (SMOM) Systems by Variation of the Chelating Phosphine and Alkane: Access to η <sup>2</sup> ,η <sup>2</sup> 'If-Alkane Rh(I), η <sup>1</sup> 'If-Alkane Rh(III) Complexes, and Alkane Encapsulation, Journal of the American Chemical Society, 2018, 140, 14958-14970.	6.6	34
808	Formation of Coinage-Metal···Fullerene Adducts. Evaluation of the Interaction Nature between Triangular Coinage Metal Complexes (M <sub><math>3 = Cu, Ag, and Au</math>) and C<sub><math>60</math> through Relativistic Density Functional Theory Calculations. Journal of Physical Chemistry C, 2018, 122, 25110-25117.</sub></sub>	1.5	21
809	Substrate Oxidation Prompted by Solvent Dissociation: The Role of Peroxo-Vanadate and Ag-Ï€ Interaction. Applied Catalysis A: General, 2018, 568, 191-201.	2.2	11
810	Benzimidazolium†and Benzimidazolilydeneâ€Capped Cyclodextrins: New Perspectives in Anion Encapsulation and Goldâ€Catalyzed Cycloisomerization of 1,6â€Enynes. Chemistry - A European Journal, 2018, 24, 17921-17926.	1.7	25
811	FALDIâ€based criterion for and the origin of an electron density bridge with an associated (3,–1) critical point on Bader's molecular graph. Journal of Computational Chemistry, 2018, 39, 2283-2299.	1.5	8
812	Computational Study of Enantioselectivity in the Asymmetric Allylation of Aldehydes with Chiral Pt(II) Phosphinite Complexes. Journal of Organic Chemistry, 2018, 83, 13911-13921.	1.7	3
813	The Structural Signs of Sweetness in Artificial Sweeteners: A Rotational Study of Sorbitol and Dulcitol. ChemPhysChem, 2018, 19, 3334-3340.	1.0	16
814	Stereospecific 1,3-H Transfer of Indenols Proceeds via Persistent Ion-Pairs Anchored by NH··Â-Ï€ Interactions. Journal of the American Chemical Society, 2018, 140, 16740-16748.	6.6	29
815	Organic phototransistors based on perylene diimide nanocrystals lacking π–π interactions. Journal of Materials Chemistry C, 2018, 6, 10597-10602.	2.7	12
816	Two chiral catalysts in action: insights into cooperativity and stereoselectivity in proline and cinchona-thiourea dual organocatalysis. Chemical Science, 2018, 9, 8738-8747.	3.7	30
817	Tetrel Bonding Interactions in Perchlorinated Cyclopenta- and Cyclohexatetrelanes: A Combined DFT and CSD Study. Molecules, 2018, 23, 1770.	1.7	11
818	Using Theory To Reinterpret the Kinetics of Monofunctional Platinum Anticancer Drugs: Stacking Matters. Journal of the American Chemical Society, 2018, 140, 14024-14027.	6.6	35
819	Trielâ€Bonded Complexes between TrR <sub>3</sub> (Tr=B, Al, Ga; R=H, F, Cl, Br, CH <sub>3</sub> ) and Pyrazine. ChemPhysChem, 2018, 19, 3122-3133.	1.0	25

#	Article	IF	CITATIONS
820	Insight into wild-type and T1372E TET2-mediated 5hmC oxidation using <i>ab initio</i> QM/MM calculations. Chemical Science, 2018, 9, 8433-8445.	3.7	27
821	Triel–hydride triel bond between ZX <sub>3</sub> (Z = B and Al; X = H and Me) and THMe <sub>3</sub> (T) Tj	ето <sub>1</sub> 11 (	0.784314 r <mark>a</mark> 14
822	Design of Chiral Bifunctional Dialkyl Sulfide Catalysts for Regioâ€; Diastereoâ€; and Enantioselective Bromolactonization. Chemistry - A European Journal, 2018, 24, 16747-16752.	1.7	34
823	A simulation study of water property changes using geometrical alteration in SPC/E. Chinese Physics B, 2018, 27, 083103.	0.7	6
824	Catalytic Reaction Mechanism in Native and Mutant Catechol- <i>O</i> -methyltransferase from the Adaptive String Method and Mean Reaction Force Analysis. Journal of Physical Chemistry B, 2018, 122, 8861-8871.	1.2	8
825	How Do Secondary Phosphine Oxides Interact with Silver Nanoclusters? Insights from Computation. Journal of Physical Chemistry C, 2018, 122, 21449-21461.	1.5	5
826	Ingenious modification of molecular structure effectively regulates excited-state intramolecular proton and charge transfer: a theoretical study based on 3-hydroxyflavone. RSC Advances, 2018, 8, 29589-29597.	1.7	42
827	Supramolecular association involving anion–π interactions in Cu(II) coordination solids: Experimental and theoretical studies. Polyhedron, 2018, 151, 381-393.	1.0	36
828	Insights into conformational changes in AlkD bound to DNA with a yatakemycin adduct from computational simulations. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	1
829	Crystal engineering, optical properties and electron density distribution of polar multicomponent materials containing sulfanilamide. CrystEngComm, 2018, 20, 3638-3646.	1.3	11
830	Stabilizing Role of Halide Ions in Endohedral [20]Silafulleranes: Insights from DFT Calculations toward Silicon Nanocages. Journal of Physical Chemistry C, 2018, 122, 12551-12558.	1.5	11
831	Local Interaction Signal Analysis Predicts Protein-Protein Binding Affinity. Structure, 2018, 26, 905-915.e4.	1.6	24
832	Hydrogenation of Multiple Bonds by Geminal Aminoboraneâ€Based Frustrated Lewis Pairs. Chemistry - A European Journal, 2018, 24, 8833-8840.	1.7	32
833	Covalent and Ionic Capacity of MOFs To Sorb Small Gas Molecules. Inorganic Chemistry, 2018, 57, 6981-6990.	1.9	55
834	Revisiting electronic nature and geometric parameters of cyclophanes and their relation with stability – DFT, QTAIM and NCI study. Computational and Theoretical Chemistry, 2018, 1135, 18-27.	1.1	4
835	Sâ< <sup>-</sup> S and Sâ< <sup>-</sup> P chalcogen bonding in solution: a cryospectroscopic study of the complexes of 2,2,4,4-tetrafluoro-1,3-dithietane with dimethyl sulfide and trimethylphosphine. New Journal of Chemistry, 2018, 42, 10563-10571.	1.4	8
836	Role of conformational dynamics in the evolution of novel enzyme function. Chemical Communications, 2018, 54, 6622-6634.	2.2	123
837	Investigating Polyoxometalate–Protein Interactions at Chemically Distinct Binding Sites. Journal of Physical Chemistry B, 2018, 122, 7219-7232.	1.2	27

#	Article	IF	CITATIONS
838	Visible-Light-Mediated Metal-Free Synthesis of Aryl Phosphonates: Synthetic and Mechanistic Investigations. Organic Letters, 2018, 20, 4164-4167.	2.4	65
839	The Role of Hydrogen Bond in the Mechanism of Autocatalytic Reaction between Acetic Anhydride and tert-Butyl Hydroperoxide. Russian Journal of General Chemistry, 2018, 88, 855-861.	0.3	1
840	Hydrogen bonding <i>versus</i> π-interactions: their key competition in sildenafil solvates. CrystEngComm, 2018, 20, 4526-4530.	1.3	9
841	Origin of stereoselectivity in the amination of alcohols using cooperative asymmetric dual catalysis involving chiral counter-ions. Chemical Science, 2018, 9, 6126-6133.	3.7	23
842	Coordination numbers in hydrated Cu(II) ions. Journal of Molecular Modeling, 2018, 24, 187.	0.8	10
843	Theoretical study of boron nitride nanotubes as drug delivery vehicles of some anticancer drugs. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	33
844	Issues Particular to Organometallic Reactions. , 2018, , 519-539.		0
845	Synthesis, structural characterization, DFT calculations and Hirshfeld surface analysis of (R)-2-((S)-2((S)-hydroxy(ferrocenyl)methyl)aziridin-1yl)butan-1-ol. Journal of Molecular Structure, 2018, 1173, 33-41.	1.8	2
846	Molecular motions in a fluxional (η6-indenyl)tricarbonylchromium hemichelate: a density functional theory molecular dynamics study. Dalton Transactions, 2018, 47, 8906-8920.	1.6	4
847	Size-dependent rate acceleration in the silylation of secondary alcohols: the bigger the faster. Chemical Science, 2018, 9, 6509-6515.	3.7	24
848	Intramolecular magnesium bonds in malonaldehyde-like systems: a critical view of the resonance-assisted phenomena. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	8
849	Insights into the N-Heterocyclic Carbene (NHC)-Catalyzed Oxidative γ-C(sp <sup>3</sup> )–H Deprotonation of Alkylenals and Cascade [4 + 2] Cycloaddition with Alkenylisoxazoles. Journal of Organic Chemistry, 2018, 83, 8543-8555.	1.7	61
850	Effect of Cosolvents DMSO and Glycerol on the Self-Assembly Behavior of SDBS and CPC: An Experimental and Theoretical Approach. Journal of Chemical & Engineering Data, 2018, 63, 3083-3096.	1.0	27
851	Chiral bisoxazoline catalyzed decarboxylative aldol reactions between β-carbonyl acids and trifluoroacetaldehyde hemiacetals as well as trifluoroacetaldehyde: the mechanism, the origin of enantioselectivity and the role of a catalyst. Organic Chemistry Frontiers, 2018, 5, 2692-2709.	2.3	18
852	Modeling Soft Supramolecular Nanostructures by Molecular Simulations. , 2018, , .		0
853	Structural Topology of Weak Non-covalent Interactions in a Layered Supramolecular Coordination Solid of Zinc Involving 3-Aminopyridine and Benzoate: Experimental and Theoretical Studies. Journal of Chemical Crystallography, 2018, 48, 156-163.	0.5	25
854	DFT exploration of [3 + 2] cycloaddition reaction of 1 <i>H</i> -phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl methacrylate. RSC Advances, 2018, 8, 27406-27416.	1.7	7
855	Tetrel bonds between PhSiF <sub>3</sub> /PhTH <sub>3</sub> (T = Si, Ge, Sn) and H <sub>3</sub> ZO (	(Z =â€ 1.0	2‰N,) Tj ETQ 4

#	Article	IF	CITATIONS
856	Strong metallophilic interactions in nickel coordination compounds. Inorganica Chimica Acta, 2018, 483, 21-25.	1.2	12
857	London dispersion as important factor for the stabilization of ( <i>Z</i> )-azobenzenes in the presence of hydrogen bonding. Beilstein Journal of Organic Chemistry, 2018, 14, 1238-1243.	1.3	14
858	Nonâ€Covalent Substrate Directed Enantioselective Heck Desymmetrization of cis â€Cyclohexâ€4â€eneâ€1,2â€d Synthesis of all cis Chiral 5â€Arylâ€cyclohexâ€3â€eneâ€1,2â€diols and Mechanistic Investigation. Advanced Synthesis and Catalysis, 2018, 360, 3760-3767.	liol: 2.1	17
859	Hybrid DFT study on non-covalent interactions and their influence on pKa's of magnesium-carboxylate complexes. Journal of Molecular Graphics and Modelling, 2018, 85, 13-24.	1.3	5
860	Unexpected diverseness on electronic density and bonding behaviours for Sc2X@C2(63751)-C86 and Sc2X@C1(63755)-C86 (X = S and O). Chemical Physics Letters, 2018, 707, 93-100.	1.2	3
861	Solvent effects on the coupling reaction of CO2 with PO catalyzed by hydroxyl imidazolium ionic liquid: Comparison of different models. Journal of CO2 Utilization, 2018, 27, 99-106.	3.3	17
862	A proton transfer network that generates deprotonated tyrosine is a key to producing reactive oxygen species in phototoxic KillerRed protein. Physical Chemistry Chemical Physics, 2018, 20, 22342-22350.	1.3	9
863	Mixed A-Cation Perovskites for Solar Cells: Atomic-Scale Insights Into Structural Distortion, Hydrogen Bonding, and Electronic Properties. Chemistry of Materials, 2018, 30, 5194-5204.	3.2	127
864	Deciphering the binding behavior of flavonoids to the cyclin dependent kinase 6/cyclin D complex. PLoS ONE, 2018, 13, e0196651.	1.1	15
865	Unveiling Noncovalent Interactions in Imidazolium, Pyrrolidinium, or Quaternary Ammonium Cation and Acetate Anion Based Protic Ionic Liquids: Structure and Spectral Characteristics. Journal of Physical Chemistry A, 2018, 122, 6225-6235.	1.1	14
866	Dual function of the boron center of BH(CO)2/BH(N2)2 in halogen- and triel-bonded complexes with hypervalent halogens. Journal of Molecular Graphics and Modelling, 2018, 84, 118-124.	1.3	8
867	The effect of the intramolecular C–Hâ⊄O interactions on the conformational preferences of bis-arylsulfones – 5-HT <sub>6</sub> receptor antagonists and beyond. RSC Advances, 2018, 8, 18672-18681.	1.7	11
868	Characterization of Nine Cancer-Associated Variants in Human DNA Polymerase κ. Chemical Research in Toxicology, 2018, 31, 697-711.	1.7	8
869	Hydrogen bond induced enhancement of Fermi resonances in N–H⋯N hydrogen bonded complexes of anilines. Physical Chemistry Chemical Physics, 2018, 20, 21557-21566.	1.3	16
870	π–π-Induced aggregation and single-crystal fluorescence anisotropy of 5,6,10b-triazaacephenanthrylene. IUCrJ, 2018, 5, 335-347.	1.0	10
871	Oenin and Quercetin Copigmentation: Highlights From Density Functional Theory. Frontiers in Chemistry, 2018, 6, 245.	1.8	18
872	Synthesis, crystal structure, computational analysis and biological properties of 1-(4-chlorobenzoyl)-3-[2-(2-{2-[3-(4-chlorobenzoyl)-thioureido]-ethoxy}ethoxy)ethyl]-thiourea and its Ni(II) and Cu(II) complexes. Journal of Molecular Structure, 2018, 1168, 153-164.	1.8	16
873	Coâ€Crystals of 2â€Aminoâ€5â€Nitropyridine Barbital with Extreme Birefringence and Large Second Harmonic Generation Effect. Chemistry - A European Journal, 2018, 24, 8727-8731.	1.7	24

#	Article	IF	CITATIONS
874	Quantifying conventional C–Hâ<ï€(aryl) and unconventional C–Hâ<ï€(chelate) interactions in dinuclear Cu( <scp>ii</scp> ) complexes: experimental observations, Hirshfeld surface and theoretical DFT study. New Journal of Chemistry, 2018, 42, 10202-10213.	1.4	72
875	Asymmetric nucleophilic fluorination under hydrogen bonding phase-transfer catalysis. Science, 2018, 360, 638-642.	6.0	137
876	Confinement induced catalytic activity in a Diels-Alder reaction: comparison among various CB[n], n = 6–8, cavitands. Journal of Molecular Modeling, 2018, 24, 228.	0.8	7
877	Cobalt-catalyzed C–H cyanations: Insights into the reaction mechanism and the role of London dispersion. Beilstein Journal of Organic Chemistry, 2018, 14, 1537-1545.	1.3	17
878	Host–guest complexes of conformationally flexible <i>C</i> -hexyl-2-bromoresorcinarene and aromatic <i>N</i> -oxides: solid-state, solution and computational studies. Beilstein Journal of Organic Chemistry, 2018, 14, 1723-1733.	1.3	9
879	Linear tricationic ionic liquids: Insights into the structural features using DFT and molecular dynamics simulation. Journal of Molecular Liquids, 2018, 271, 96-104.	2.3	17
880	A series of 3D lanthanide coordination polymers decorated with a rigid 3,5-pyridinedicarboxylic acid linker: syntheses, structural diversity, DFT study, Hirshfeld surface analysis, luminescence and magnetic properties. Dalton Transactions, 2018, 47, 12318-12336.	1.6	54
881	Characterizing Hydrogen-Bond Interactions in Pyrazinetetracarboxamide Complexes: Insights from Experimental and Quantum Topological Analyses. Inorganic Chemistry, 2018, 57, 9775-9778.	1.9	3
882	Synthesis of Unique Phosphazane Macrocycles via Steric Activation of C–N Bonds. Inorganic Chemistry, 2018, 57, 10993-11004.	1.9	9
883	Two-dimensional silicon carbide structure under uniaxial strains, electronic and bonding analysis. Computational Materials Science, 2018, 151, 288-295.	1.4	26
884	Modulation of an Anagostic Interaction in SiPSi-Type Pincer Platinum Complexes. Organometallics, 2018, 37, 3581-3587.	1.1	8
885	Topology and Equilibrium Analysis of the Monovalent Aluminum Compound Al <sub>4</sub> Cp* <sup>Ph</sup> <sub>4</sub> . Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2018, 644, 454-464.	0.6	0
886	Helicenes as Molecular Tweezers in the Formation of Cationâ~'Ï€ Complexes. Bonding and Circular Dichroism Properties from Relativistic DFT Calculations. ChemPhysChem, 2018, 19, 2321-2330.	1.0	9
887	The effects of cation–i̇́€ and anion–i̇́€ interactions on halogen bonds in the [N⋯X⋯N]+ complexes: A comprehensive theoretical study. Journal of Molecular Graphics and Modelling, 2018, 84, 134-144.	1.3	12
888	Unexpected reactivity of graphene oxide with DBU and DMF. Journal of Materials Chemistry A, 2018, 6, 12637-12646.	5.2	12
889	Confinement of H <sub>2</sub> O and EtOH to enhance CO <sub>2</sub> capture in MIL-53(Al)-TDC. Dalton Transactions, 2018, 47, 9459-9465.	1.6	20
890	Steroid–Fullerene Hybrids from Epiandrosterone: Synthesis, Characterization and Theoretical Study. European Journal of Organic Chemistry, 2018, 2018, 4512-4522.	1.2	9
891	Concerted Albeit Not Pericyclic Cycloadditions: Understanding the Mechanism of the (4+3) Cycloaddition between Nitrones and 1,2â€Diazaâ€1,3â€dienes. European Journal of Organic Chemistry, 2019, 2019, 391-400.	1.2	4

#	Article	IF	CITATIONS
892	An unusual werner type clathrate of Mn(II) benzoate involving energetically significant weak C H⋯C contacts: A combined experimental and theoretical study. Journal of Molecular Structure, 2019, 1175, 130-138.	1.8	29
893	Investigation of potential anti-malarial lead candidate 2-(4-fluorobenzylthio)-5-(5-bromothiophen-2-yl)-1,3,4-oxadiazole: Insights from crystal structure, DFT, QTAIM and hybrid QM/MM binding energy analysis. Journal of Molecular Structure, 2019, 1175, 230-240.	1.8	23
894	Crystal structure, non-covalent interaction and molecular docking studies of product: 2-(phenyl-sulfonyl)phthalazin-1(2H)-one. Journal of Molecular Structure, 2019, 1175, 219-229.	1.8	10
895	Assessment of the chitosan-functionalized graphene oxide as a carrier for loading thioguanine, an antitumor drug and effect of urea on adsorption process: Combination of DFT computational and molecular dynamics simulation studies. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2487-2497.	2.0	31
896	Synthesis and characterization of azathiaethers macrocyclic rings decorated with one or two 2-pyridylmethyl fragments. Journal of Molecular Structure, 2019, 1176, 54-65.	1.8	1
897	Evaluation of the aggregation process in a mixture of propofol and benzocaine. Physical Chemistry Chemical Physics, 2019, 21, 3537-3544.	1.3	0
898	Competition between σ-hole pnicogen bond and π-hole tetrel bond in complexes of CF <sub>2</sub> =CFZH <sub>2</sub> (Z = P, As, and Sb). Molecular Physics, 2019, 117, 251-259.	0.8	15
899	A review on the information content of the pair density as a tool for the description of the electronic properties in molecular systems. International Journal of Quantum Chemistry, 2019, 119, e25763.	1.0	8
900	Case study of 2-vinyloxypyridine: Quantitative assessment of the intramolecular C H⋯N hydrogen bond energy and its contribution to the one-bond 13C1H coupling constant. Journal of Molecular Structure, 2019, 1176, 73-85.	1.8	9
901	Intermolecular C–Hâ<¯O and n → Ï€* and short intramolecular σ → Ï€* interactions in the molybdenum(0) tetracarbonyl complex of a very twisted 14-membered tetraazaannulene macrocyclic ligand: structural and computational studies. CrystEngComm, 2019, 21, 5222-5226.	1.3	10
902	Microhydration Structures of Protonated Oxazole. Journal of Physical Chemistry A, 2019, 123, 7637-7650.	1.1	10
903	Influence of Non-Covalent Interactions in the <i>Exo</i> - and Regioselectivity of Aza-Diels–Alder Reactions: Experimental and DFT Calculations. Journal of Organic Chemistry, 2019, 84, 10825-10831.	1.7	11
904	Two Geometrical Isomers of a 1D Coordination Polymer: Rationalization by Theoretical Calculations and Variation of Electrical Properties with the Change in Binding Mode of Dicarboxylate Linker. Crystal Growth and Design, 2019, 19, 5819-5828.	1.4	19
905	Can 2-X-Ethanols Form Intramolecular Hydrogen Bonds?. Journal of Physical Chemistry A, 2019, 123, 7651-7660.	1.1	12
906	Effects of N-oxidation on the molecular and crystal structures and properties of isocinchomeronic acid, its metal complexes and their supramolecular architectures: experimental, CSD survey, solution and theoretical approaches. RSC Advances, 2019, 9, 25382-25404.	1.7	15
907	Antiproliferative evaluation and supramolecular association in Mn(II) and Zn(II) bipyridine complexes: Combined experimental and theoretical studies. Journal of Inorganic Biochemistry, 2019, 200, 110803.	1.5	37
908	A comprehensive DFT study on the sensing abilities of cyclic oligothiophenes ( <i>n</i> CTs). New Journal of Chemistry, 2019, 43, 14120-14133.	1.4	45
909	Violation of Electrostatic Rules: Shifting the Balance between Pnicogen Bonds and Lone Pairâ^ï€ Interactions Tuned by Substituents. Journal of Physical Chemistry A, 2019, 123, 7288-7295.	1.1	11

#	Article	IF	CITATIONS
910	Genoprotection by complexation: The case of Phyllanthus orbicularis K extract. Computational and Theoretical Chemistry, 2019, 1164, 112555.	1.1	1
911	Hierarchical Noncovalent Interactions between Molecules Stabilize Multicomponent Cocrystals. Crystal Growth and Design, 2019, 19, 4802-4809.	1.4	14
912	Cis/Trans Energetics in Epoxide, Thiirane, Aziridine and Phosphirane Containing Cyclopentanols: Effects of Intramolecular OHâ⊄O, S, N and P Contacts. Molecules, 2019, 24, 2523.	1.7	2
913	A combined experimental and theoretical analysis of the solid-state supramolecular self-assembly of N-(2,4-dichlorophenyl)-1-naphthamide: Synthesis, anticholinesterase potential and molecular docking analysis. Journal of Molecular Structure, 2019, 1197, 458-470.	1.8	15
914	A Germylene Supported by Two 2â€Pyrrolylphosphane Groups as Precursor to PGeP Pincer Squareâ€Planar Groupâ€10 Metal(II) and Tâ€Shaped Gold(I) Complexes. Chemistry - A European Journal, 2019, 25, 12423-124	30. <sup>1.7</sup>	26
915	Effect of Enhanced Electron Withdrawal on the Cohesion of Cr-Pd Hemichelates. European Journal of Inorganic Chemistry, 2019, 2019, 3301-3308.	1.0	5
916	Stabilization of Pancake Bonding in (TCNQ) 2 .â^' Dimers in the Radicalâ€Anionic Salt (Nâ^'CH 3 â^'2â€NH 2) Tj E	TQ <sub>Q</sub> Q 0 0	rgBJT /Overlo
917	Effect of the Si, Al and B doping on the sensing behaviour of carbon nanotubes toward ethylene oxide: a computational study. Molecular Simulation, 2019, 45, 1384-1394.	0.9	8
918	X-Ray Diffraction and Theoretical Calculation–Supported Formation of Polymorphic Cocrystals Discovered Through Thermal Methods: A Case Study. Journal of Pharmaceutical Sciences, 2019, 108, 3340-3347.	1.6	19
919	The reaction of phenoxatellurine with single-electron oxidizers revisited. New Journal of Chemistry, 2019, 43, 12754-12766.	1.4	13
920	Quantum mechanistic study of furan and 2-methylfuran hydrodeoxygenation on molybdenum and tungsten sulfide clusters. Journal of Molecular Modeling, 2019, 25, 237.	0.8	8
921	Stereodivergent Construction of Tertiary Fluorides in Vicinal Stereogenic Pairs by Allylic Substitution with Iridium and Copper Catalysts. Journal of the American Chemical Society, 2019, 141, 13066-13073.	6.6	155
922	Scandium catalysed stereoselective thio-allylation of allenyl-imidates. Chemical Communications, 2019, 55, 9669-9672.	2.2	3
923	Uncovering the Molecular Interactions in the Catalytic Loop That Modulate the Conformational Dynamics in Protein Tyrosine Phosphatase 1B. Journal of the American Chemical Society, 2019, 141, 12634-12647.	6.6	40
924	Deciphering the Allosterically Driven Conformational Ensemble in Tryptophan Synthase Evolution. Journal of the American Chemical Society, 2019, 141, 13049-13056.	6.6	49
925	Mn(I) and Fe(II)/PN(H)P Catalysts for the Hydrogenation of Ketones: A Comparison by Experiment and Calculation. Advanced Synthesis and Catalysis, 2019, 361, 4691-4706.	2.1	42
926	A Benchmark of Density Functional Approximations For Thermochemistry and Kinetics of Hydride Reductions of Cyclohexanones. ChemistryOpen, 2019, 8, 788-806.	0.9	7
927	Exfoliation of Ti2C and Ti3C2 Mxenes from bulk trigonal phases of titanium carbide: A theoretical prediction. Solid State Communications, 2019, 299, 113657.	0.9	30

ARTICLE IF CITATIONS Elucidating the origin of selectivity of [3 + 2]-cycloaddition reactions between thioketone and 928 0.8 8 carbohydrate-derived nitrones by the DFT. Journal of Molecular Modeling, 2019, 25, 209. Theoretical studies of perfluorochemicals (PFCs) adsorption mechanism on the carbonaceous 4.2 23 surface. Chemosphere, 2019, 235, 606-615. Enhance the efficiency of 5-fluorouracil targeted delivery by using a prodrug approach as a novel strategy for prolonged circulation time and improved permeation. International Journal of 930 2.6 15 Pharmaceutics, 2019, 568, 118491. Bioinspired Functional Catechol Derivatives through Simple Thiol Conjugate Addition. Chemistry - A European Journal, 2019, 25, 12367-12379. Halogen Bonding and Cooperative Effects in Chlorine Clathrate: Ab Initio Periodic Study. Journal of 932 1.56 Physical Chemistry C, 2019, 123, 24793-24806. Unraveling the protonation site of oxazole and solvation with hydrophobic ligands by infrared 1.3 photodissociation spectroscopy. Physical Chemistry Chemical Physics, 2019, 21, 15157-15166. Fast and Accurate Quantum Crystallography: From Small to Large, from Light to Heavy. Journal of 934 2.1 48 Physical Chemistry Letters, 2019, 10, 6973-6982. A Complex Containing Four Magnesium Atoms and Two Mg–Mg Bonds Behaving as an Electride. 1.0 European Journal of Inorganic Chemistry, 2019, 2019, 4105-4111. The Electron Density Distribution in Crystals of η<sup>6</sup>–[1,4–dihydrospiró(2<i>H</i>–3,1–benzoxazine–2,1â€2–cyclohexane)]tricarbonylchr**om**ium(0)8 936 Experiment <i>vs</i> Molecular Invariom. ChemistrySelect, 2019, 4, 10976-10982. Antiproliferative evaluation and supramolecular association involving electrostatically enhanced π-Ï€ interaction in isostructural coordination solids of Mn(II), Co(II) and  $\overline{Z}n(II)$  chlorobenzoates: 1.2 Experimental and theoretical studies. Inorganica Chimica Acta, 2019, 498, 119161. Nitrogenated holey graphene (C2N) surface as highly selective electrochemical sensor for ammonia. 938 2.369 Journal of Molecular Liquids, 2019, 296, 111929. Tailoring of graphene quantum dots for toxic heavy metals detection. Applied Physics A: Materials 1.1 Science and Processing, 2019, 125, 1. Indirect influence of alkyl substituent on sigma-hole interactions: The case study of antimony(III) 940 diphenyldithiophosphates with covalent Sb-S and non-covalent Sba<sup>-</sup>S pnictogen bonds. Polyhedron, 1.0 18 2019, 173, 114126. Silver-based monomer and coordination polymer with organic thiocyanate ligand: Structural, computational and antiproliferative activity study. Polyhedron, 2019, 173, 114132. 941 1.0 The Naâ€"O bond in sodium fenamate. Acta Crystallographica Section B: Structural Science, Crystal 942 0.54 Engineering and Materials, 2019, 75, 766-774. Insight into Isothiourea atalyzed Enantioselective Addition of Saturated Esters to Iminium Ions. 943 Chemistry - an Asian Journal, 2019, 14, 4322-4327. Internal Motions and Sulfur Hydrogen Bonding in Methyl 3-Mercaptopropionate. Journal of Physical 944 1.1 8 Chemistry A, 2019, 123, 984Ó-9849. Crystal Structure and (Non)linear Optical Properties of a Cyanuric Acid Isoniazid <1/1&gt; 945 Co-crystal: Shortcomings of Phase Matching Determination from Powdered Samples. Crystal Growth 1.4 and Design, 2019, 19, 6831-6836.

#	Article	IF	CITATIONS
946	Reaction Mechanism of Li and Mg Carbenoid Cyclopropanations: Metal-ï€ and ïƒ Interactions. ACS Omega, 2019, 4, 19452-19461.	1.6	5
947	Intramolecular H-Bond Is Formed in 2-Fluorophenol and 2-Fluorothiophenol, but It May Not Be the Main Pathway of the JFH Coupling Constant Transmission. Journal of Physical Chemistry A, 2019, 123, 10072-10078.	1.1	11
948	Diastereodivergent Asymmetric 1,3â€Dipolar Cycloaddition of Azomethine Ylides and βâ€Fluoroalkyl Vinylsulfones: Low Copper(II) Catalyst Loading and Theoretical Studies. Angewandte Chemie, 2019, 131, 16790-16796.	1.6	10
949	Online dualâ€rate decentralized structural identification for wireless sensor networks. Structural Control and Health Monitoring, 2019, 26, e2453.	1.9	11
950	Mechanism of Coupling of Alcohols and Amines To Generate Aldimines and H <sub>2</sub> by a Pincer Manganese Catalyst. ACS Catalysis, 2019, 9, 1662-1669.	5.5	62
951	Diastereodivergent Asymmetric 1,3â€Dipolar Cycloaddition of Azomethine Ylides and βâ€Fluoroalkyl Vinylsulfones: Low Copper(II) Catalyst Loading and Theoretical Studies. Angewandte Chemie - International Edition, 2019, 58, 16637-16643.	7.2	43
952	Phenomenal Observation of Attractive Intermolecular CHâ‹⁻HC Interaction in a Mercury (II) Complex: An Experimental and Firstâ€Principles Study. ChemistrySelect, 2019, 4, 10246-10253.	0.7	10
953	Hydrogen Bonding versus Hâ^'H Interactions in Pillar[n]arenes. ChemistrySelect, 2019, 4, 9354-9359.	0.7	3
954	TriQuinoline. Nature Communications, 2019, 10, 3820.	5.8	25
955	Aluminum adsorption on graphene: Theoretical study of dispersion effects. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950019.	1.8	3
956	Labeling IL-18 with alkaloids: toward the use of cytokines as carrier molecules in chemotherapy. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	1
957	Hydride–Rhodium(III)- <i>N</i> -Heterocyclic Carbene Catalyst for Tandem Alkylation/Alkenylation via C–H Activation. ACS Catalysis, 2019, 9, 9372-9386.	5.5	11
958	Experimental and theoretical study of Pb⋯S and Pb⋯O σ-hole interactions in the crystal structures of Pb( <scp>ii</scp> ) complexes. CrystEngComm, 2019, 21, 6018-6025.	1.3	20
959	Tuning receptors for the encapsulation of beryllium <sup>2+</sup> . Physical Chemistry Chemical Physics, 2019, 21, 19660-19666.	1.3	8
960	A noncovalent interaction insight onto the concerted metallation deprotonation mechanism. Physical Chemistry Chemical Physics, 2019, 21, 20486-20498.	1.3	17
961	Supramolecular association involving antiparallel COâ√CO and anion–π contacts in Co(II) and Mn(II) complexes involving 2,5-pyridinedicarboxylate: Anticancer evaluation and theoretical studies. Inorganica Chimica Acta, 2019, 498, 119108.	1.2	17
962	Diastereoselective diazenyl formation: the key for manganese-catalysed alcohol conversion into ( <i>E</i> )-alkenes. Dalton Transactions, 2019, 48, 14122-14127.	1.6	18
963	Electron density learning of non-covalent systems. Chemical Science, 2019, 10, 9424-9432.	3.7	92

# ARTICLE

964

The Role for the Weak Interaction on the Stabilization of Copper-Containing Complex: DFT Investigation of Noncovalent Interactions in Ternary-Cu(II) (DA)(AA) Complexes (DA = Diamine and AA =) Tj ETQq0 9.0 rgBT /Qverlock 10

964	1874-1882.		0 -	/
965	2Ch–2N square and hexagon interactions: a combined crystallographic data analysis and computational study. Physical Chemistry Chemical Physics, 2019, 21, 21568-21576.	1.:	3	17
966	Chiral Phosphoric Acid-Catalyzed Enantioselective Direct Arylation of Iminoquinones: A Case Study of the Model Selectivity. Journal of Organic Chemistry, 2019, 84, 13473-13482.	1.7	7	7
967	Charge-transfer interactions between fullerenes and a mesoporous tetrathiafulvalene-based metal–organic framework. Beilstein Journal of Nanotechnology, 2019, 10, 1883-1893.	1.	5	24
968	Experimental study of X-ray charge density and the selection of reference points for a source function in η6-(2-methyl-1,4-dihydro-2H-3,1-benzoxazine)tricarbonylchromium(0). Mendeleev Communications, 2019, 29, 346-348.	0.	.6	8
969	A Modular Approach to Phosphorescent π-Extended Heteroacenes. Inorganic Chemistry, 2019, 58, 13323-13336.	1.9	9	20
970	Dealing with Hydrogen Bonding on the Conformational Preference of 1,3-Aminopropanols: Experimental and Molecular Dynamics Approaches. Journal of Physical Chemistry A, 2019, 123, 8583-8594.	1.	1	9
971	Observation of a weak intra-residue C5 hydrogen-bond in a dipeptide containing Gly-Pro sequence. Journal of Chemical Physics, 2019, 151, 104309.	1.:	2	8
972	Solid-state supramolecular architectures of a series of Hg( <scp>ii</scp> ) halide coordination compounds based on hydroxyl-substituted Schiff base ligands. CrystEngComm, 2019, 21, 6301-6312.	1.;	3	9
973	Hydroxyl-functionalized pyrazolium ionic liquids to catalyze chemical fixation of CO2: Further benign reaction condition for the single-component catalyst. Journal of Molecular Liquids, 2019, 293, 111479.	2.	3	18
974	NCI-ELMO: A New Method To Quickly and Accurately Detect Noncovalent Interactions in Biosystems. Journal of Chemical Theory and Computation, 2019, 15, 6456-6470.	2.	3	21
975	Tailoring of the self-assembled structures and optical waveguide behaviour of arylaminofluorenone derivatives. Dyes and Pigments, 2019, 171, 107780.	2.	0	2
976	Conformational preferences of N-acetyl-N′-methylprolineamide in different media: a 1H NMR and theoretical investigation. New Journal of Chemistry, 2019, 43, 1757-1763.	1.4	4	5
977	Supramolecular association in Cu(II) coordination complexes involving energetically significant NOâ‹īNO l€â€"hole interaction and cooperative l€-stacked ternary assembly: Experimental and theoreti studies. Inorganica Chimica Acta, 2019, 488, 159-169.	cal 1.:	2	33
978	Werner type clathrates involving guest benzoic acid and benzoate in discrete Mn(II) hosts: Experimental and theoretical studies. Polyhedron, 2019, 159, 387-399.	1.0	0	28
979	One pot stimuli-responsive linear waterborne polyurethanes via Diels-Alder reaction. Progress in Organic Coatings, 2019, 130, 31-43.	1.9	9	22
980	Origin of the Immiscibility of Alkanes and Perfluoroalkanes. Journal of the American Chemical Society, 2019, 141, 3489-3506.	6.	6	45
981	Structures, metallophilic interactions and electronic excitation energy of linear metal chain complexes PdmPtn[PH2(CH2PH)m+n-2CH2PH2]3, a theoretical investigation. Computational and Theoretical Chemistry, 2019, 1151, 24-30.	1,:	1	0

IF ARTICLE CITATIONS # Selective photoisomerisation of 2-chloromalonaldehyde. Journal of Chemical Physics, 2019, 150, 982 1.2 3 034305. Bis(6-diphenylphosphinoacenaphth-5-yl)telluride as a ligand toward coinage metal chlorides. Dalton Transactions, 2019, 48, 2635-2645. 1.6 An enantioconvergent halogenophilic nucleophilic substitution (S <sub>N</sub> 2X) reaction. 984 6.0 100 Science, 2019, 363, 400-404. A computational study on ligand assisted <i>vs.</i> ligand participation mechanisms for CO<sub>2</sub> hydrogenation: importance of bifunctional ligand based catalysts. Physical Chemistry Chemical Physics, 2019, 21, 3932-3941.

Enhancing effects of π-hole tetrel bonds on the Ïf-hole interactions in complexes involving F2TO (T = Si,) Ţj ÆTQq0 Q 0 rgBT /O

**CITATION REPORT** 

987	A Computational Study on the Stereo- and Regioselective Formation of the C4α–C6′ Bond of Tethered Catechin Moieties by an Exhaustive Search of the Transition States. Journal of Organic Chemistry, 2019, 84, 2840-2849.	1.7	3
988	The beryllium bond. Advances in Inorganic Chemistry, 2019, 73, 73-121.	0.4	36
989	Asymmetric, Nearly Barrierless C(sp <sup>3</sup> )–H Activation Promoted by Easily-Accessible <i>N-</i> Protected Aminosulfoxides as New Chiral Ligands. ACS Catalysis, 2019, 9, 2532-2542.	5.5	59
990	New rhenium-tricarbonyl complexes bearing halogen-substituted bidentate ligands: structural, computational and Hirshfeld surfaces studies. CrystEngComm, 2019, 21, 77-93.	1.3	10
991	A mechanistic investigation into N-heterocyclic carbene (NHC) catalyzed umpolung of ketones and benzonitriles: is the cyano group better than the classical carbonyl group for the addition of NHC?. Organic Chemistry Frontiers, 2019, 6, 523-531.	2.3	4
992	H-Bonded anion–anion complexes in fentanyl citrate polymorphs and solvates. Chemical Communications, 2019, 55, 115-118.	2.2	26
993	Solvent-driven structural topology involving energetically significant intra- and intermolecular chelate ring contacts and anticancer activities of Cu( <scp>ii</scp> ) phenanthroline complexes involving benzoates: experimental and theoretical studies. RSC Advances, 2019, 9, 16339-16356.	1.7	47
994	A new type of halogen bond involving multivalent astatine: an <i>ab initio</i> study. Physical Chemistry Chemical Physics, 2019, 21, 15310-15318.	1.3	39
995	New olefin metathesis catalyst bearing N-mesitylimidazole and nitrate ligands – Synthesis, activity, and performance in aqueous media. Journal of Organometallic Chemistry, 2019, 896, 154-161.	0.8	3
996	How does the pH influences the Ruâ€NO coordination compounds?. International Journal of Quantum Chemistry, 2019, 119, e25999.	1.0	2
997	Enhanced π-back-donation resulting in the <i>trans</i> labilization of a pyridine ligand in an N-heterocyclic carbene (NHC) Pd <sup>II</sup> precatalyst: a case study. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 941-950.	0.2	13
998	"Like–like―tetrel bonding interactions between Sn centres: a combined <i>ab initio</i> and CSD study. Dalton Transactions, 2019, 48, 11208-11216.	1.6	18
999	Methylene spacer regulated variation in molecular and crystalline architectures of cobalt( <scp>iii</scp> ) complexes with reduced Schiff base ligands: a combined experimental and	1.6	21

theoretical study. Dalton Transactions, 2019, 48, 11433-11447.

#	Article	IF	CITATIONS
1000	Electrostatic potential and non-covalent interactions analysis for the design of selective 5-HT7 ligands. Journal of Molecular Graphics and Modelling, 2019, 91, 130-139.	1.3	8
1001	Iodine-Catalyzed Nazarov Cyclizations. Journal of Organic Chemistry, 2019, 84, 7587-7605.	1.7	32
1002	On the nature of organic electron density transfer complexes within molecular electron density theory. Organic and Biomolecular Chemistry, 2019, 17, 6478-6488.	1.5	12
1003	Mechanistic investigation-inspired activation mode of DBU and the function of the α-diazo group in the reaction of the α-amino ketone compound and EDA: [DBU-H] <sup>+</sup> -DMF-H <sub>2</sub> O and α-diazo as strong N-terminal nucleophiles. Organic Chemistry Frontiers, 2019, 6, 2678-2686.	2.3	2
1004	Copper(I)â€Catalyzed Enantioconvergent Borylation of Racemic Benzyl Chlorides Enabled by Quadrantâ€byâ€Quadrant Structure Modification of Chiral Bisphosphine Ligands. Angewandte Chemie, 2019, 131, 11229-11234.	1.6	13
1005	Gibbs energy of complex formation – combining infrared spectroscopy and vibrational theory. International Reviews in Physical Chemistry, 2019, 38, 115-148.	0.9	22
1006	Sulfur as a hydrogen bond donor in the gas phase: Rotational spectroscopic and computational study of 3-mercaptopropionic acid. Journal of Molecular Spectroscopy, 2019, 362, 1-7.	0.4	5
1007	Understanding electronic effects on carboxylate-assisted C–H activation at ruthenium: the importance of kinetic and thermodynamic control. Faraday Discussions, 2019, 220, 386-403.	1.6	23
1008	Mechanistic Study on the Asymmetric Synthesis of the Wielandâ€Miescher Ketone and Analogs. ChemCatChem, 2019, 11, 4064-4071.	1.8	5
1009	Copper(I)â€Catalyzed Enantioconvergent Borylation of Racemic Benzyl Chlorides Enabled by Quadrantâ€byâ€Quadrant Structure Modification of Chiral Bisphosphine Ligands. Angewandte Chemie - International Edition, 2019, 58, 11112-11117.	7.2	53
1010	Influence of the solvent in the electronic excitation of aromatic alcohols: Excited state IR-UV of propofol(H2O)8. Journal of Chemical Physics, 2019, 150, 214306.	1.2	2
1011	Theory and practice of modeling van der Waals interactions in electronic-structure calculations. Chemical Society Reviews, 2019, 48, 4118-4154.	18.7	114
1012	Mechanism of atom economical conversion of alcohols and amines to amides using Fe( <scp>ii</scp> ) pincer catalyst. An outer-sphere metal–ligand pathway or an inner-sphere elimination pathway?. RSC Advances, 2019, 9, 17479-17489.	1.7	3
1013	Increasing the Potential of the Auristatin Cancer-Drug Family by Shifting the Conformational Equilibrium. Molecular Pharmaceutics, 2019, 16, 3600-3608.	2.3	7
1014	Cu(II) and Co(II) coordination solids involving unconventional parallel nitrile(π)‒nitrile(π) and energetically significant cooperative hydrogen bonding interactions: Experimental and theoretical studies. Journal of Molecular Structure, 2019, 1195, 733-743.	1.8	31
1015	An Improved Class of Phosphite-Oxazoline Ligands for Pd-Catalyzed Allylic Substitution Reactions. ACS Catalysis, 2019, 9, 6033-6048.	5.5	18
1016	Understanding the affinity of bis-exTTF macrocyclic receptors towards fullerene recognition. Physical Chemistry Chemical Physics, 2019, 21, 11670-11675.	1.3	12
1017	A regression approach to accurate interaction energies using topological descriptors. Computational and Theoretical Chemistry, 2019, 1159, 23-26.	1.1	16

#	Article	IF	CITATIONS
1018	Probing non-covalent interactions of phosphine and arsine derivatives: an energy decomposition analysis using localized molecular orbitals. Structural Chemistry, 2019, 30, 2191-2204.	1.0	0
1019	A Universal Quantitative Descriptor of the Dispersion Interaction Potential. Angewandte Chemie - International Edition, 2019, 58, 9758-9769.	7.2	41
1020	Deciphering the Origin of Enantioselectivity on the Cis-Cyclopropanation of Styrene with Enantiopure Di-chloro,Di-gold(I)-SEGPHOS Carbenoids Generated from Propargylic Esters. Journal of Organic Chemistry, 2019, 84, 7664-7673.	1.7	6
1021	An MEDT study of the mechanism and selectivities of the [3+2] cycloaddition reaction of tomentosin with benzonitrile oxide. International Journal of Quantum Chemistry, 2019, 119, e25980.	1.0	21
1022	Energetically favorable anti-electrostatic hydrogen bonded cationic clusters in Ni(II) 3,5-dimethylpyrazole complexes: Anticancer evaluation and theoretical studies. Polyhedron, 2019, 168, 113-126.	1.0	36
1023	Dibenzyl Disulfide Adsorption on Cationic Exchanged Faujasites: A DFT Study. Nanomaterials, 2019, 9, 715.	1.9	16
1024	Water Docking Bias in [4]Helicene. Angewandte Chemie, 2019, 131, 11379-11383.	1.6	0
1025	Water Docking Bias in [4]Helicene. Angewandte Chemie - International Edition, 2019, 58, 11257-11261.	7.2	11
1026	Insights into N-Heterocyclic Carbene-Catalyzed Oxidative α-C(sp <sup>3</sup> )–H Activation of Aliphatic Aldehydes and Cascade [2 + 2] Cycloaddition with Ketimines. Journal of Organic Chemistry, 2019, 84, 6117-6125.	1.7	42
1027	A d <sup>10</sup> Ag( <scp>i</scp> ) amine–borane σ-complex and comparison with a d <sup>8</sup> Rh( <scp>i</scp> ) analogue: structures on the Î <sup>1</sup> to Î <sup>2</sup> :Î <sup>2</sup> continuum. Dalton Transactions, 2019, 48, 9776-9781.	1.6	12
1028	Nonbonding interaction analyses on PVDF/[BMIM][BF4] complex system in gas and solution phase. Journal of Molecular Modeling, 2019, 25, 131.	0.8	21
1029	Superstrong Noncovalent Interface between Melamine and Graphene Oxide. ACS Applied Materials & Interfaces, 2019, 11, 17068-17078.	4.0	18
1030	On the importance of antiparallel π–π interactions in the solid state of isatin-based hydrazides. New Journal of Chemistry, 2019, 43, 8122-8131.	1.4	23
1031	Cyclometalated Au <sup>III</sup> Complexes for Cysteine Arylation in Zinc Finger Protein Domains: towards Controlled Reductive Elimination. Chemistry - A European Journal, 2019, 25, 7628-7634.	1.7	53
1032	Seeking the best model for non-covalent interactions within the crystal structure of meloxicam. Computational and Theoretical Chemistry, 2019, 1157, 47-53.	1.1	10
1033	Theoretical study of C-arylations with aryl halides to determine the reaction mechanism, the effect of substituents and heteroatoms. Physical Chemistry Chemical Physics, 2019, 21, 10163-10170.	1.3	6
1034	Thermodynamic, structural and dynamic properties of ionic liquids [C4mim][CF3COO], [C4mim][Br] in the condensed phase, using molecular simulations. RSC Advances, 2019, 9, 13677-13695.	1.7	4
1035	Water-mediated weakening of inter-ionic interactions in aqueous mixtures of ionic liquid: An investigation combining quantum chemical calculations and molecular dynamics simulations. Chemical Physics, 2019, 524, 31-39.	0.9	6

#	Article	IF	CITATIONS
1036	Structure and Dynamics in Amino Acid Choline-Based Ionic Liquids: A Combined QTAIM, NCI, DFT, and Molecular Dynamics Study. Journal of Physical Chemistry B, 2019, 123, 4070-4084.	1.2	30
1037	Comparative studies on the effect of CB[8] on the charge transfer interaction. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	2
1038	Theoretical characterization of (CuF) (n = 1–12) clusters. Computational and Theoretical Chemistry, 2019, 1157, 28-33.	1.1	4
1039	Catalytically Active Species in Copper/DiPPAMâ€Catalyzed 1,6â€Asymmetric Conjugate Addition of Dialkylzinc to Dienones: A Computational Overview. ChemCatChem, 2019, 11, 4108-4115.	1.8	6
1040	Energetically significant unconventional π-π contacts involving fumarate in a novel coordination polymer of Zn(II): In-vitro anticancer evaluation and theoretical studies. Inorganica Chimica Acta, 2019, 493, 1-13.	1.2	47
1041	Lone pairâ< <sup>−</sup> Ï€ interaction <i>versus</i> σ-hole appearance in metal-bonded halogens. CrystEngComm, 2019, 21, 2929-2939.	1.3	3
1042	New insights into the dihydrogen bonds (MHδâ~ʾ··Ĥδ+X) in CpM(PMe3)(L)2H···HX (M=Cr, Mo, W; L=PMe	3, CO;) Tj   1.0	ETQq0 0 0 rg
1043	Theoretical insights into the sensing mechanism of a series of terpyridine-based chemosensors for TNP. Chemical Physics Letters, 2019, 725, 45-51.	1.2	15
1044	A Solution Processed Ultrathin Molecular Dielectric for Organic Field-Effect Transistors. ACS Applied Electronic Materials, 2019, 1, 485-493.	2.0	4
1045	Four-component relativistic <sup>31</sup> P NMR calculations for <i>trans</i> -platinum( <scp>ii</scp> ) complexes: importance of the solvent and dynamics in spectral simulations. Dalton Transactions, 2019, 48, 8076-8083.	1.6	18
1046	Metal-ligand bifunctional based Mn-catalysts for CO2 hydrogenation reaction. Molecular Catalysis, 2019, 468, 109-116.	1.0	15
1047	Theoretical and Crystallographic Study of Lead(IV) Tetrel Bonding Interactions. Chemistry - A European Journal, 2019, 25, 6007-6013.	1.7	22
1048	Structural Characterization and Biological Evaluation of 18â€Nor―ent â€labdane Diterpenoids from Grazielia gaudichaudeana. Chemistry and Biodiversity, 2019, 16, e1800644.	1.0	8
1049	When does a hydrogen bond become a <scp>van der Waals</scp> interaction? a topological answer. Journal of Computational Chemistry, 2019, 40, 937-943.	1.5	17
1050	Complexes featuring N-heterocyclic carbenes with bowl-shaped wingtips. Comptes Rendus Chimie, 2019, 22, 299-309.	0.2	5
1051	Influence of carbon nanostructure and oxygen moieties on dopamine adsorption and charge transfer kinetics at glassy carbon surfaces. Electrochimica Acta, 2019, 304, 221-230.	2.6	21
1052	Theoretical ab Initio Study on Cooperativity Effects between Nitro Ï€â€hole and Halogen Bonding Interactions. ChemPhysChem, 2019, 20, 1135-1144.	1.0	21
1053	Experimental and theoretical study on cetylpyridinium dipicrylamide – A promising ion-exchanger for cetylpyridinium selective electrodes. Journal of Molecular Structure, 2019, 1187, 77-85.	1.8	28

#	Article	IF	CITATIONS
1054	Transmetallation of bis(6-diphenylphosphinoxy-acenapth-5-yl)mercury with tin tetrachloride, antimony trichloride and bismuth trichloride. Dalton Transactions, 2019, 48, 5585-5594.	1.6	11
1055	Role of London Dispersion Interactions in Ga-Substituted Dipnictenes. Organometallics, 2019, 38, 1640-1647.	1.1	32
1056	Study of the effect of the ligand structure on the catalytic activity of Pd@ ligand decorated halloysite: Combination of experimental and computational studies. Applied Organometallic Chemistry, 2019, 33, e4891.	1.7	57
1057	The role of viscosity in various dynamical processes of different fluorophores in ionic liquid— cosolvent mixtures: a femtosecond fluorescence upconversion study. Photochemical and Photobiological Sciences, 2019, 18, 1359-1372.	1.6	4
1058	Integrated Computational Study of the Cu-Catalyzed Hydration of Alkenes in Water Solvent and into the Context of an Artificial Metallohydratase. ACS Catalysis, 2019, 9, 4616-4626.	5.5	10
1059	Deeper Insights into Conformational Analysis of <i>cis</i> Butene and 1-Alkenes as Monomers and Dimers: QTAIM, NCI, and DFT Approach. Journal of Chemistry, 2019, 2019, 1-13.	0.9	1
1060	Steric Clashes, Doughnuts and Exploding Cigars: Some Comments on Nonâ€Covalent Interactions. ChemistrySelect, 2019, 4, 4238-4243.	0.7	6
1061	Insights into NHC-catalyzed oxidative α-C(sp <sup>3</sup> )–H activation of aliphatic aldehydes and cascade [2 + 3] cycloaddition with azomethine imines. Catalysis Science and Technology, 2019, 9, 2514-2522.	2.1	48
1062	Rotational Signatures of Dispersive Stacking in the Formation of Aromatic Dimers. Angewandte Chemie, 2019, 131, 3140-3145.	1.6	14
1063	Classical and Quantum Mechanical Calculations of the Stacking Interaction of Nd <sup>III</sup> Complexes with Regular and Mismatched DNA Sequences. Journal of Physical Chemistry B, 2019, 123, 3219-3231.	1.2	5
1064	Computational Modelling Study on the Pseudoazurin TypeÂ1 Cu Site. , 2019, , .		0
1065	Why electrostatically enhanced thiourea is better than Schreiner's thiourea in both catalytic activity and regioselectivity?. Organic Chemistry Frontiers, 2019, 6, 1821-1831.	2.3	7
1066	Carbon Nanotubes Conjugated with Triazoleâ€Based Tetrathiafulvaleneâ€Type Receptors for C <sub>60</sub> Recognition. ChemPlusChem, 2019, 84, 730-739.	1.3	4
1067	Chiral phosphoric acid-catalyzed asymmetric C(sp <sup>3</sup> )–H functionalization of biomass-derived 2,5-dimethylfuran <i>via</i> two sequential Cope-type rearrangements. Organic Chemistry Frontiers, 2019, 6, 1162-1167.	2.3	21
1068	Analysis of energies of halogen and hydrogen bonding interactions in the solid state structures of vanadyl Schiff base complexes. RSC Advances, 2019, 9, 4789-4796.	1.7	18
1069	Diverse structural assemblies of U-shaped hydrazinyl-sulfonamides: experimental and theoretical analysis of non-covalent interactions stabilizing solid state conformations. CrystEngComm, 2019, 21, 1780-1793.	1.3	12
1070	Formation of small clusters of NaCl dihydrate in the gas phase. New Journal of Chemistry, 2019, 43, 4342-4348.	1.4	15
1071	Understanding the Molecular Mechanism of the Rearrangement of Internal Nitronic Ester into Nitronorbornene in Light of the MEDT Study. Molecules, 2019, 24, 462.	1.7	16

#	Article	IF	CITATIONS
1072	Rotational Signatures of Dispersive Stacking in the Formation of Aromatic Dimers. Angewandte Chemie - International Edition, 2019, 58, 3108-3113.	7.2	26
1073	Ambiguous Role of N → Sn Coordinated Stannylene: Lewis Base or Acid?. Organometallics, 2019, 38, 816-828.	1.1	15
1074	Intrinsic stability enhancement and ionic migration reduction by fluorinated cations incorporated in hybrid lead halide perovskites. Journal of Materials Chemistry C, 2019, 7, 5299-5306.	2.7	17
1075	Influence of nanopore density on ethylene/acetylene separation by monolayer graphene. Physical Chemistry Chemical Physics, 2019, 21, 6126-6132.	1.3	15
1076	A Molecular Electron Density Theory Study of the Chemoselectivity, Regioselectivity, and Diastereofacial Selectivity in the Synthesis of an Anticancer Spiroisoxazoline derived from α-Santonin. Molecules, 2019, 24, 832.	1.7	39
1077	Size and shape effects on complexes of fullerenes with carbon nanorings: C50 and C76 as [10]CPP and [6]CPPA guests. Structural Chemistry, 2019, 30, 647-656.	1.0	2
1078	Axial Ligand Effects of Ruâ€BDA Complexes in the O–O Bond Formation via the I2M Bimolecular Mechanism in Water Oxidation Catalysis. European Journal of Inorganic Chemistry, 2019, 2019, 2101-2108.	1.0	26
1079	Nature and Strength of M–H···S and M–H···Se (M = Mn, Fe, & Co) Hydrogen Bond. Journal of Phys Chemistry A, 2019, 123, 2227-2236.	sical 1.1	23
1080	Exploring Cycloreversion Reaction of Cyclobutane Pyrimidine Dimers Quantum Mechanically. Journal of Physical Chemistry A, 2019, 123, 2025-2039.	1.1	4
1081	The base-catalyzed keto-enol tautomerism of chrysophanol anthrone. A DFT investigation of the base-catalyzed reaction. Molecular Simulation, 2019, 45, 716-723.	0.9	2
1082	Transition metal complexes of antimony centered ligands based upon acenaphthyl scaffolds. Coordination non-innocent or not?. Dalton Transactions, 2019, 48, 4504-4513.	1.6	18
1083	Insights into the biotransformation of 2,4,6-trinitrotoluene by the old yellow enzyme family of flavoproteins. A computational study. Physical Chemistry Chemical Physics, 2019, 21, 11589-11598.	1.3	5
1084	Unravelling the mechanism and the origin of the selectivity of the [3 + 2] cycloaddition reaction between electrophilic nitrone and nucleophilic alkene. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	11
1085	Laboratory Evolution of GH11 Endoxylanase Through DNA Shuffling: Effects of Distal Residue Substitution on Catalytic Activity and Active Site Architecture. Frontiers in Bioengineering and Biotechnology, 2019, 7, 350.	2.0	20
1086	Chloranilate bridged dinuclear copper( <scp>ii</scp> ) complexes: <i>syn</i> – <i>anti</i> geometry tuned by the steric factor and supramolecular interactions. CrystEngComm, 2019, 21, 6886-6893.	1.3	9
1087	Unraveling the regioselectivity of odd electron halogen bond formation using electrophilicity index and chemical hardness parameters. Physical Chemistry Chemical Physics, 2019, 21, 26580-26590.	1.3	15
1088	The control effects of different scaffolds in chiral phosphoric acids: a case study of enantioselective asymmetric arylation. Catalysis Science and Technology, 2019, 9, 6482-6491.	2.1	7
1089	Why hydroxy-proline improves the catalytic power of the peptidoglycan <i>N</i> -deacetylase enzyme: insight from theory. Physical Chemistry Chemical Physics, 2019, 21, 23338-23345.	1.3	13

#	Article	IF	Citations
1090	Origins of stereoselectivity in uncatalyzed and ZnBr2-catalyzed Diels–Alder reactions of a chiral sulfinylquinone. Organic and Biomolecular Chemistry, 2019, 17, 8756-8767.	1.5	0
1091	Can sulfur-containing molecules solvate/ionize HCl? Solid state solvation of HCl on/in methanethiol clusters/nanoparticles. Journal of Chemical Physics, 2019, 151, 194309.	1.2	0
1092	Theoretical Study of the Antioxidant Activity of Quercetin Oxidation Products. Frontiers in Chemistry, 2019, 7, 818.	1.8	48
1093	A Universal Quantitative Descriptor of the Dispersion Interaction Potential. Angewandte Chemie, 2019, 131, 9860-9871.	1.6	8
1094	Self-Assembly of Partially Oxidized Pillar[5]arene into Fibrous Structures. Journal of Physical Chemistry B, 2019, 123, 10562-10568.	1.2	4
1095	A combinatorial approach to improving the performance of azoarene photoswitches. Beilstein Journal of Organic Chemistry, 2019, 15, 2753-2764.	1.3	53
1096	Chemical bonding in Period 2 homonuclear diatomic molecules: a comprehensive relook. Journal of Chemical Sciences, 2019, 131, 1.	0.7	6
1097	Diethylaminophenyl-based Schiff base Cu( <scp>ii</scp> ) and V( <scp>iv</scp> ) complexes: experimental and theoretical studies and cytotoxicity assays. New Journal of Chemistry, 2019, 43, 18832-18842.	1.4	22
1098	Intracluster proton transfer in protonated benzonitrile–(H <sub>2</sub> O) <sub>nâ‰<b>g</b></sub> nanoclusters: hydrated hydronium core for <i>n</i> ≥ 2. Physical Chemistry Chemical Physics, 2019, 21, 25226-25246.	1.3	14
1099	Confined toluene within InOF-1: CO <sub>2</sub> capture enhancement. RSC Advances, 2019, 9, 32864-32872.	1.7	11
1100	Stabilization of two conformers <i>via</i> intra- or inter-molecular hydrogen bonds in a dinuclear vanadium( <scp>v</scp> ) complex with a pendant Schiff base: theoretical insight. RSC Advances, 2019, 9, 35165-35175.	1.7	19
1101	Intramolecular Hydrogen Bond Activation of Azaâ€Methylene Imines in Hydrogen Bond Bifunctional Catalysis – A Density Functional Theory Study. European Journal of Organic Chemistry, 2019, 2019, 574-581.	1.2	10
1102	Supramolecular association in Cu(II) and Co(II) coordination complexes of 3,5-dimethylpyrazole: Experimental and theoretical studies. Inorganica Chimica Acta, 2019, 484, 133-141.	1.2	36
1103	A novel oxalato bridged supramolecular ternary complex of Cu(II) involving energetically significant ï€-hole interaction: Experimental and theoretical studies. Inorganica Chimica Acta, 2019, 487, 354-361.	1.2	37
1104	Understanding and Quantifying London Dispersion Effects in Organometallic Complexes. Accounts of Chemical Research, 2019, 52, 258-266.	7.6	117
1105	Synthesis, physicochemical and quantum chemical studies on a new organic NLO crystal: Cinnamoylproline. Journal of Molecular Structure, 2019, 1180, 826-838.	1.8	12
1106	Experimental and theoretical assessment of the interactions of ionic liquids (ILs) with fluoridated compounds (HF, R-F) in organic medium. Journal of Molecular Liquids, 2019, 276, 779-793.	2.3	8
1107	Observation of an anionâ<ānion interaction in a square planar copper(II) Schiff base complex: DFT study and CSD analysis. Inorganica Chimica Acta, 2019, 487, 465-472.	1.2	11

#	Article	IF	CITATIONS
1108	In Silico Design of New Inhibitors Against Hemagglutinin of Influenza. Journal of Physical Chemistry B, 2019, 123, 582-592.	1.2	8
1109	Neighboring Protonation Unveils Lewis Acidity in the B <sub>3</sub> NO <sub>2</sub> Heterocycle. Journal of the American Chemical Society, 2019, 141, 1546-1554.	6.6	35
1110	Towards the Design of Optically Active Thiophene Sâ€Oxides using Quantum Chemistry. Chemistry - A European Journal, 2019, 25, 2840-2851.	1.7	2
1111	Nonbonding pairs in cyclic thioethers: Electrostatic modeling and ab initio calculations for complexes of 2,5â€dihydrothiophene, thietane, and thiirane with hydrogen fluoride. International Journal of Quantum Chemistry, 2019, 119, e25885.	1.0	2
1112	[3 + 2] cycloaddition reaction ofN,N′cyclic azomethine imines toward highly electronâ€deficient nitroalkenes: A molecular electron density theory study. Journal of Physical Organic Chemistry, 2019, 32, e3925.	0.9	4
1113	Tetranuclear Mn <sup>II</sup> /Zn <sup>II</sup> and Novel Azidoâ€Bridged Chairâ€Shaped Heptanuclear Cd <sup>II</sup> Compounds: The Effect of Metal Ion and Coordination Mode of the Azide Group on the Structure of the Products. European Journal of Inorganic Chemistry, 2019, 2019, 262-270.	1.0	15
1114	The Effect of Donor Additives on the Stability and Structure of 5â€Diphenylphosphinoacenaphthâ€6â€yllithium. European Journal of Inorganic Chemistry, 2019, 2019, 712-720.	1.0	8
1115	Comparison of Ïfâ€fÏ€â€Hole Tetrel Bonds between TH <sub>3</sub> F/F <sub>2</sub> TO and H <sub>2</sub> CX (X=O, S, Se). ChemPhysChem, 2019, 20, 627-635.	1.0	28
1116	Tuning the physicochemical properties of the single-walled boron nitride nanotube by covalent grafting of triazolium-based [MTZ][X1–3] (X1–3= NTf2â^', TfOâ^' and BF4â^') ionic liquids in the gas phase and solvent media: A quantum chemical approach. Journal of Molecular Liquids, 2019, 277, 726-737.	2.3	2
1117	Understanding the Reactivity and Selectivity of Fluxional Chiral DMAP atalyzed Kinetic Resolutions of Axially Chiral Biaryls. Chemistry - A European Journal, 2019, 25, 4452-4459.	1.7	11
1118	A triple alkoxo bridged dinuclear cobalt(III) complex mimicking phosphatase and showing ability to degrade organic dye contaminants by photocatalysis. Journal of Organometallic Chemistry, 2019, 883, 52-64.	0.8	13
1119	2,5-Furandicarboxylic acid as a linker for lanthanide coordination polymers: the role of heteroaromatic ï€â€"ï€ stacking and hydrogen bonding. New Journal of Chemistry, 2019, 43, 2179-2195.	1.4	41
1120	Combination of experimental and theoretical methods to explore the amino-functionalized pyrazolium ionic liquids: An efficient single-component catalyst for chemical fixation of CO2 under mild conditions. Molecular Catalysis, 2019, 466, 37-45.	1.0	32
1121	Theoretical analysis of the adsorption of ammonia–borane and their dehydrogenation products on the (001) surface of TiC and ZrC. Surface Science, 2019, 680, 95-106.	0.8	9
1122	GPUs as boosters to analyze scalar and vector fields in quantum chemistry. International Journal of Quantum Chemistry, 2019, 119, e25671.	1.0	28
1123	Influence of fluorination on alcohol hydrogen-bond donating properties. , 2019, , 301-324.		2
1124	Aurophilicity and Photoluminescence of (6â€Diphenylpnicogenoacenaphthâ€5â€yl)gold Compounds. European Journal of Inorganic Chemistry, 2019, 2019, 647-659.	1.0	12
1125	Halogen bonds and metal bonds involving superalkalies M2OCN/M2NCO (M = Li, Na) complexes. Structural Chemistry, 2019, 30, 965-977.	1.0	13

#	Article	IF	CITATIONS
1126	An acetonitrile-solvated cocrystal of piroxicam and succinic acid with co-existing zwitterionic and non-ionized piroxicam molecules. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 29-37.	0.2	8
1127	Influence of remote intramolecular hydrogen bonding on the acidity of hydroxyâ€1,4â€benzoquinonederivatives: A DFT study. Journal of Physical Organic Chemistry, 2019, 32, e3919.	0.9	17
1128	Designing Reactions with Post-Transition-State Bifurcations: Asynchronous Nitrene Insertions into C–C σ Bonds. CheM, 2019, 5, 227-236.	5.8	28
1129	Insights into the Structure and Function of a Chiral Conjugateâ€Baseâ€6tabilized BrÃ,nsted Acid Catalyst. European Journal of Organic Chemistry, 2019, 2019, 486-492.	1.2	18
1130	On the cation–΀ capabilities of small all sp <sup>2</sup> arbon host structures. Evaluation of [6.8] <sub>3</sub> cyclacene from relativistic DFT calculations. International Journal of Quantum Chemistry, 2019, 119, e25811.	1.0	5
1131	Controllable and scalable synthesis of hollow-structured porous aromatic polymer for selective adsorption and separation of HMF from reaction mixture of fructose dehydration. Chemical Engineering Journal, 2019, 358, 467-479.	6.6	29
1132	Seven and eight-coordinate Fe(III) complexes containing pre-organized ligand 1,10-phenanthroline-2,9-dicarboxylic acid: Solvent effects, supramolecular interactions and DFT calculations. Inorganica Chimica Acta, 2019, 484, 264-275.	1.2	15
1133	Synthesis, crystal structure, and non-covalent interactions in ethyl 4-hydrazinobenzoate hydrochloride. Journal of Molecular Structure, 2019, 1177, 363-370.	1.8	4
1134	Linking Low-Coordinate Ge(II) Centers via Bridging Anionic N-Heterocyclic Olefin Ligands. Inorganic Chemistry, 2020, 59, 1592-1601.	1.9	15
1135	Density functional theory study towards investigating the adsorption properties of the Î <sup>3</sup> -Fe2O3 nanoparticles as a nanocarrier for delivery of Flutamide anticancer drug. Adsorption, 2020, 26, 925-939.	1.4	12
1136	DFT study of non-covalent interaction mechanisms of solvents with GO surfaces and the solvent-mediated GO interaction. Applied Surface Science, 2020, 499, 143926.	3.1	7
1137	Interaction of (G4)2 and (X4)2 DNA quadruplexes with Cu+, Ag+ and Au+ metal cations: a quantum chemical calculation on structural, energetic and electronic properties. Structural Chemistry, 2020, 31, 465-484.	1.0	4
1138	Synthesis, crystal structure, and non-covalent interactions in 4-hydrazinobenzoic acid hydrochloride. Journal of Molecular Structure, 2020, 1201, 127154.	1.8	1
1139	Rationalising Supramolecular Hydrogelation of Bisâ€Ureaâ€Based Gelators through a Multiscale Approach. ChemPlusChem, 2020, 85, 267-276.	1.3	9
1140	Synthesis, structural and DFT interpretation of a Schiff base assisted Mn(III) derivative. Journal of Molecular Structure, 2020, 1199, 126985.	1.8	3
1141	Mechanistic study of the formation of quercetine cycloadducts under microwave conditions: a theoretical approach. Molecular Physics, 2020, 118, .	0.8	2
1142	Halogen interactions in dinuclear copper(II) 2,4-dibromophenoxyacetate – crystal structure and quantum chemical calculations. Journal of Molecular Structure, 2020, 1202, 127227.	1.8	5
1143	The effect of a double n(O) → Ï€â^—(C = O) intramolecular interaction on the stability of 3-nitrophthalic acid. Structural Chemistry, 2020, 31, 305-317.	1.0	2

#	Article	IF	CITATIONS
1144	Understanding the origin of the enantioselectivity and the mechanism of the asymmetric reduction of ketimine generated from acetophenone with oxazaborolidine catalyst. Structural Chemistry, 2020, 31, 253-261.	1.0	7
1145	DFT studies on the interactions of pristine, Al and Ga-doped boron nitride nanosheets with CH3X (X=F,) Tj ETQq1	1_0,78432 1.8	l4 <sub>3</sub> rgBT /O∨
1146	Synthesis and structural studies of hexafluorophosphate-based organic salts: A combined experimental and computational analysis. Journal of Molecular Structure, 2020, 1202, 127337.	1.8	1
1147	Nature of C 60 and C 70 fullerene encapsulation in a porphyrin―and metalloporphyrinâ€based cage: Insights from dispersionâ€corrected density functional theory calculations. International Journal of Quantum Chemistry, 2020, 120, e26080.	1.0	15
1148	Energetically significant antiparallel π-stacking contacts in Co(II), Ni(II) and Cu(II) coordination compounds of pyridine-2,6-dicarboxylates: Antiproliferative evaluation and theoretical studies. Inorganica Chimica Acta, 2020, 501, 119233.	1.2	26
1149	Synthesis, crystal structure, hydrogen bonding interactions analysis of novel acyl thiourea derivative. Journal of Physical Organic Chemistry, 2020, 33, e4016.	0.9	2
1150	Hybrid and bioactive cocrystals of pyrazinamide with hydroxybenzoic acids: Detailed study of structure, spectroscopic characteristics, other potential applications and noncovalent interactions using SAPT. Journal of Molecular Structure, 2020, 1202, 127316.	1.8	47
1151	Keteniminium Salts as Key Intermediates for the Efficient Synthesis of 3â€Aminoâ€Indoles and â€Benzofurans. Helvetica Chimica Acta, 2020, 103, e1900217.	1.0	5
1152	Unconventional Reactivity of Ethynylbenziodoxolone Reagents and Thiols: Scope and Mechanism. Chemistry - A European Journal, 2020, 26, 2386-2394.	1.7	28
1153	Experimental and theoretical probing of the physicochemical properties of ionic liquids composed of [Bn-DBU]+ cation and various anions. Journal of Molecular Structure, 2020, 1202, 127226.	1.8	12
1154	Zn(II) and Co(II) derivatives anchored with scorpionate precursor: Antiproliferative evaluation in human cancer cell lines. Journal of Inorganic Biochemistry, 2020, 202, 110881.	1.5	4
1155	A combined experimental and computational study of a supramolecular assembly based on cationic zinc(II)-ethanesulfonate. Journal of Molecular Structure, 2020, 1202, 127206.	1.8	1
1156	Phenoxylation of Alkynes through Mono―and Dual Activation Using Group 11 (Cu, Ag, Au) Catalysts. European Journal of Inorganic Chemistry, 2020, 2020, 1123-1134.	1.0	7
1157	Formaldehyde adsorption on a hydrogenated gallium nitride monolayer: A density functional theory study. Applied Surface Science, 2020, 506, 144944.	3.1	13
1158	A DFT Study on the Redox Active Behavior of Carbene and Pyridine Ligands in the Oxidative and Reductive Quenching Cycles of Ruthenium Photoredox Catalysts. Catalysts, 2020, 10, 80.	1.6	5
1159	<i>cis</i> alkenes stabilized by intramolecular sulphurâ<ï€ interactions. Chemical Communications, 2020, 56, 814-817.	2.2	5
1160	Mechanistic insights into Cu-catalyzed enantioselective Friedel–Crafts reaction between indoles and 2-aryl-N-sulfonylaziridines. Catalysis Science and Technology, 2020, 10, 1117-1124.	2.1	2
1161	How does the acidic milieu interfere in the capability of ruthenium nitrosyl complexes to release nitric oxide?. New Journal of Chemistry, 2020, 44, 773-779.	1.4	6

#	Article	IF	CITATIONS
1162	Computational and Experimental Analysis on the Conformational Preferences of Anticancer Saponin OSW-1. Journal of Organic Chemistry, 2020, 85, 339-344.	1.7	2
1163	A one-pot route to <i>N</i> -acyl ureas: a formal four-component hydrolytic reaction involving aminonitrones and isocyanide dibromides. New Journal of Chemistry, 2020, 44, 1253-1262.	1.4	7
1164	Perethylated pillar[n]arenes versus pillar[n]arenes: theoretical perspectives. Journal of Molecular Modeling, 2020, 26, 3.	0.8	3
1165	Atomic Decomposition Scheme of Noncovalent Interactions Applied to Host–Guest Assemblies. Journal of Chemical Information and Modeling, 2020, 60, 268-278.	2.5	50
1166	Theoretical investigation of excited-state proton transfer (ESPT) for 2,5-bis(2-benzothiazolyl)hydroquinone: single or double?. Molecular Physics, 2020, 118, e1705413.	0.8	4
1167	Molecular and supramolecular recognition patterns in ternary copper(II) or zinc(II) complexes with selected rigid-planar chelators and a synthetic adenine-nucleoside. Journal of Inorganic Biochemistry, 2020, 203, 110920.	1.5	5
1168	Do Carbon Nanoâ€onions Behave as Nanoscopic Faraday Cages? A Comparison of the Reactivity of C <sub>60</sub> , C <sub>240</sub> , C <sub>60</sub> @C <sub>240</sub> , Li <sup>+</sup> @C <sub>60</sub> , Li <sup>+</sup> @C <sub>240</sub> , and Li <sup>+</sup> @C <sub>60</sub> @C <sub>240</sub> . Chemistry - A European Journal, 2020, 26, 804-808.	1.7	12
1169	Three-phenyl transfer in palladium-catalyzed C C coupling reactions by triarylbismuths: A mechanistic study. Molecular Catalysis, 2020, 482, 110649.	1.0	0
1170	Axial Chirality around N–P Bonds Induced by Complexation between E(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> (E = B, Al) and an <i>N</i> Phosphine Oxide-Substituted Imidazolinylidene: A Key Intermediate in the Catalytic Phosphinoylation of CO <sub>2</sub> . Journal of Organic Chemistry, 2020, 85, 14333-14341.	1.7	9
1171	Metal–organic architectures driven by a multifunctional 6-aminouracil spacer: structures, noncovalent interactions, and conductivity. CrystEngComm, 2020, 22, 829-840.	1.3	7
1172	NCIPLOT4 Guide for Biomolecules: An Analysis Tool for Noncovalent Interactions. Journal of Chemical Information and Modeling, 2020, 60, 6-10.	2.5	24
1173	Closest-Packing Water Monolayer Stably Intercalated in Phyllosilicate Minerals under High Pressure. Langmuir, 2020, 36, 618-627.	1.6	7
1174	Copigmentation evidence of oenin with phenolic compounds: A comparative study of spectrographic, thermodynamic and theoretical data. Food Chemistry, 2020, 313, 126163.	4.2	19
1175	A physicochemical and conformational study of co-solvent effect on the molecular interactions between similarly charged protein surfactant (BSA-SDBS) system. Journal of Chemical Thermodynamics, 2020, 142, 106022.	1.0	32
1176	Supramolecular architecture constructed from the hemidirected lead(II) complex with N'-(4-hydroxybenzylidene)isonicotinohydrazide. Inorganica Chimica Acta, 2020, 502, 119350.	1.2	25
1177	Keteniminium Salts: Reactivity and Propensity toward Electrocyclization Reactions. Journal of Organic Chemistry, 2020, 85, 449-463.	1.7	7
1178	Energetically significant unconventional O Hâ⊂Ï€ contacts involving discrete guest (H2O)8 clusters in a fumarato bridged polymeric supramolecular host of Ni(II) phenanthroline: Antiproliferative evaluation and theoretical studies. Polyhedron, 2020, 176, 114266.	1.0	23
1179	A Topological Data Analysis perspective on noncovalent interactions in relativistic calculations. International Journal of Quantum Chemistry, 2020, 120, e26133.	1.0	16

~		~	
		REPO	<b>DT</b>
$\sim$	IIAI	IVE FV	

#	Article	IF	CITATIONS
1180	Theoretical Study of the Mechanism of Catalytic Enanteoselective N–H and O–H Insertion Reactions. Journal of Physical Chemistry A, 2020, 124, 2-11.	1.1	8
1181	Evolution of Bonding during the Insertion of Anionic Ibuprofen into Model Cell Membranes. Journal of Physical Chemistry B, 2020, 124, 79-90.	1.2	21
1182	Substituent Effect on Conformational Preferences in Ground and Excited States of Selected Schiff Bases: An Insight from Theoretical Calculations. Journal of Physical Chemistry A, 2020, 124, 63-73.	1.1	6
1183	Non-covalent interactions between epinephrine and nitroaromatic compounds: A DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117827.	2.0	22
1184	Metal–Halogen Bonding Seen through the Eyes of Vibrational Spectroscopy. Materials, 2020, 13, 55.	1.3	26
1185	Molecular insight into the selective binding between human telomere Gâ€quadruplex and a negatively charged stabilizer. Clinical and Experimental Pharmacology and Physiology, 2020, 47, 892-902.	0.9	7
1186	The Adsorption of Chlorofluoromethane on Pristine, Alâ€, Gaâ€, Pâ€, and Asâ€doped Boron Nitride Nanotubes: A PBCâ€DFT, NBO, and QTAIM Study. ChemistrySelect, 2020, 5, 12115-12124.	0.7	28
1187	Impact of the Novel Z-Acceptor Ligand Bis{( <i>ortho</i> -diphenylphosphino)phenyl}zinc (ZnPhos) on the Formation and Reactivity of Low-Coordinate Ru(0) Centers. Inorganic Chemistry, 2020, 59, 15606-15619.	1.9	9
1188	Insight into the role of weak interactions on optoelectronic properties of LiGaTe2-chalcopyrite under pressure effect: DFT-D3, NCI and QTAIM investigations. Physica B: Condensed Matter, 2020, 599, 412463.	1.3	15
1189	Harnessing the Efficacy of 2-Pyridone Ligands for Pd-Catalyzed (β/γ)-C(sp <sup>3</sup> )–H Activations. Journal of Organic Chemistry, 2020, 85, 13228-13238.	1.7	22
1190	Intramolecular Spodium Bonds in Zn(II) Complexes: Insights from Theory and Experiment. International Journal of Molecular Sciences, 2020, 21, 7091.	1.8	41
1191	Intermolecular interactions in antipyrine-like derivatives 2-halo- <i>N</i> -(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1 <i>H</i> -pyrazol-4-yl)benzamides: X-ray structure, Hirshfeld surface analysis and DFT calculations. New Journal of Chemistry, 2020, 44, 19541-19554.	1.4	23
1192	Core–Satellite Gold Nanoparticle Complexes Grown by Inert Gas-Phase Condensation. Journal of Physical Chemistry C, 2020, 124, 24441-24450.	1.5	8
1193	DFT investigation on Lewis base-catalyzed Lewis acid-mediated reactions: hypervalent silicon species as chiral organocatalysts in (direct) aldol reactions. New Journal of Chemistry, 2020, 44, 19288-19293.	1.4	0
1194	The adsorption of chlorofluoromethane on pristine, and Al- and Ga-doped boron nitride nanosheets: a DFT, NBO, and QTAIM study. Journal of Molecular Modeling, 2020, 26, 287.	0.8	35
1195	Copper-Catalyzed Enantioselective Radical 1,4-Difunctionalization of 1,3-Enynes. Journal of the American Chemical Society, 2020, 142, 18014-18021.	6.6	109
1196	The simultaneous recognition mechanism of cations and anions using macrocyclic–iodine structures: insights from dispersion-corrected DFT calculations. Physical Chemistry Chemical Physics, 2020, 22, 23795-23803.	1.3	2
1197	Recurrent Ï€(arene)â<¯Ï€(chelate ring) motifs in four trinuclear Cull2MII (M = Cd/Zn) complexes derived from an unsymmetrical N2O2 donor ligand: structural and theoretical investigations. CrystEngComm, 2020, 22, 7673-7683.	1.3	7

	CITATION REF	PORT	
#	Article	IF	CITATIONS
1198	Mechanistic Studies Inform Design of Improved Ti(salen) Catalysts for Enantioselective [3 + 2] Cycloaddition. Journal of the American Chemical Society, 2020, 142, 18471-18482.	6.6	32
1199	Structures and internal dynamics of diphenylether and its aggregates with water. Physical Chemistry Chemical Physics, 2020, 22, 27966-27978.	1.3	7
1200	Targeting the Rich Conformational Landscape of N â€Allylmethylamine Using Rotational Spectroscopy and Quantum Mechanical Calculations. ChemPhysChem, 2020, 21, 2515-2522.	1.0	9
1201	Therapeutic potential of graphitic carbon nitride as a drug delivery system for cisplatin (anticancer) Tj ETQq1 1 0.7	'84314 rgl 1.5	BT/Overlact
1202	Adsorption properties study of boron nitride fullerene for the application as smart drug delivery agent of anti-cancer drug hydroxyurea by density functional theory. Journal of Molecular Liquids, 2020, 318, 114315.	2.3	53
1203	Supramolecular architectures of Mn(NCS)2 complexes with N'-(1-(pyridin-4-yl)ethylidene)picolinohydrazide and N'-(phenyl(pyridin-4-yl)methylene)isonicotinohydrazide. Polyhedron, 2020, 190, 114776.	1.0	9
1204	A C(π-hole)⋯Cl–Zn tetrel interaction driving a metal–organic supramolecular assembly. CrystEngComm, 2020, 22, 6979-6982.	1.3	2
1205	Optical properties of photodynamic therapy drugs in different environments: the paradigmatic case of temoporfin. Physical Chemistry Chemical Physics, 2020, 22, 16956-16964.	1.3	17
1206	The interplay and the formation of σ-hole in the π···LiX and pseudo-π···LiX (XÂ=ÂF, Cl and CN) lithium bor involving unsaturated and homocyclic hydrocarbons. Computational and Theoretical Chemistry, 2020, 1186, 112899.	nds 1.1	2
1207	Push-pull nitronates in the [3+2] cycloaddition with nitroethylene: Molecular Electron Density Theory study. Journal of Molecular Graphics and Modelling, 2020, 97, 107549.	1.3	11
1208	The equilibrium molecular structure of 3-methyl-4-nitro- and 4-methyl-3-nitrofuroxans by gas-phase electron diffraction and coupled cluster calculations. Journal of Molecular Structure, 2020, 1222, 128856.	1.8	7
1209	The formation of H···X hydrogen bond, C···X carbon-halide or Si···X tetrel bonds on the silylene-halogen dimers (X = F or Cl): intermolecular strength, molecular orbital interactions and prediction of covalency. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	6
1210	Synthesis, Structure and Bonding Analysis of the Zwitterionic PPP-Pincer Complex (6-Ph2P-Ace-5-)2P(O)AuCl2. Crystals, 2020, 10, 564.	1.0	1
1211	Real-Space Approach to the Reaction Force: Understanding the Origin of Synchronicity/Nonsynchronicity in Multibond Chemical Reactions. Journal of Physical Chemistry A, 2020, 124, 1959-1972.	1.1	12
1212	Protobranching as repulsion-induced attraction: a prototype for geminal stabilization. Physical Chemistry Chemical Physics, 2020, 22, 16998-17006.	1.3	1
1213	Transmetallation of Bis(6â€diphenylphosphinoacenaphthâ€5â€yl)â€Mercury and â€Tributyltin with Precious Metal Chlorides. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2020, 646, 856-865.	0.6	4
1214	Analyzing the N–H+…π interactions of protonated tryptophan and phenylalkylamines using QTAIM, NCI, and NBO. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	6
1215	Adsorption of cytarabine and gemcitabine anticancer drugs on the BNNT surface: DFT and GD3-DFT approaches. Adsorption, 2020, 26, 1365-1384.	1.4	5

#	Article	IF	CITATIONS
1216	A physiological examination of the antioxidant ability of super tocopherol derivatives. Structural Chemistry, 2020, 31, 2313-2319.	1.0	3
1217	A MEDT computational study of the mechanism, reactivity and selectivity of non-polar [3+2] cycloaddition between quinazoline-3-oxide and methyl 3-methoxyacrylate. Journal of Molecular Modeling, 2020, 26, 328.	0.8	6
1218	Bis(silanetellurone) with C–H···Te Interaction. Inorganic Chemistry, 2020, 59, 17811-17821.	1.9	9
1219	<sup>±</sup> ï€â€Hole Interactions: A Comparative Investigation Based on Boronâ€Containing Molecules. ChemistrySelect, 2020, 5, 13223-13231.	0.7	12
1220	Origin of Stereoselectivity in FLP-Catalyzed Asymmetric Hydrogenation of Imines. ACS Catalysis, 2020, 10, 14290-14301.	5.5	24
1221	A new spodium bond driven coordination polymer constructed from mercury( <scp>ii</scp> ) azide and 1,2-bis(pyridin-2-ylmethylene)hydrazine. New Journal of Chemistry, 2020, 44, 21100-21107.	1.4	21
1222	Gas-Phase Binding Energies and Dissociation Dynamics of 1-Alkyl-3-Methylimidazolium Tetrafluoroborate Ionic Liquid Clusters. Journal of Physical Chemistry A, 2020, 124, 10181-10198.	1.1	8
1223	Interconvertible Hydrochlorothiazide–Caffeine Multicomponent Pharmaceutical Materials: A Solvent Issue. Crystals, 2020, 10, 1088.	1.0	13
1224	Bicyclic Guanidine-Catalyzed Asymmetric Cycloaddition Reaction of Anthrones—Bifunctional Binding Modes and Origin of Stereoselectivity. Journal of Organic Chemistry, 2020, 85, 15139-15153.	1.7	7
1225	Two conformational polymorphs of 4-methylhippuric acid. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 1077-1091.	0.5	3
1226	Unconventional formation of a 1D-chain of H-bonded water molecules in bipyridine-based supramolecular hexameric hosts of isostructural coordination compounds of Co(II) and Zn(II): Antiproliferative evaluation and theoretical studies. Polyhedron, 2020, 191, 114809.	1.0	20
1227	Synthesis and Reactivity of Spirocarbocycles as Scaffolds for Nucleoside Analogues. Journal of Organic Chemistry, 2020, 85, 14989-15005.	1.7	1
1228	Bis(6â€diphenylphosphinoâ€acenaphthâ€5â€yl)sulfoxide: A New Ligand for Late Transition Metal Complexes. European Journal of Inorganic Chemistry, 2020, 2020, 3829-3836.	1.0	2
1229	2-Oxaadamant-1-yl Ureas as Soluble Epoxide Hydrolase Inhibitors: <i>In Vivo</i> Evaluation in a Murine Model of Acute Pancreatitis. Journal of Medicinal Chemistry, 2020, 63, 9237-9257.	2.9	14
1230	Unraveling the binding and micellization behavior of dioctylsulfosuccinate Sodium Salt with vitamin B1 and B6: A physiochemical and computational study. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2020, 605, 125324.	2.3	4
1231	What is the driving force behind molecular triangles and their guests? A quantum chemical perspective about host–guest interactions. Physical Chemistry Chemical Physics, 2020, 22, 19213-19222.	1.3	2
1232	Exploration of the Interaction Strength at the Interface of Anionic Chalcogen Anchors and Gold (111)-Based Nanomaterials. Nanomaterials, 2020, 10, 1237.	1.9	1
1233	From Capsule to Helix: Guest-Induced Superstructures of Chiral Macrocycle Crystals. Journal of the American Chemical Society, 2020, 142, 15823-15829.	6.6	18

#	Article	IF	CITATIONS
1234	Recurrent ï€â€"ï€ stacking motifs in three new 4,5-dihydropyrazolyl–thiazole–coumarin hybrids: X-ray characterization, Hirshfeld surface analysis and DFT calculations. New Journal of Chemistry, 2020, 44, 14592-14603.	1.4	54
1235	Self-association process of tetracycline antibiotic in different aqueous solutions: a joint experimental study and molecular dynamics simulation. Journal of the Iranian Chemical Society, 2020, 17, 2997-3007.	1.2	4
1236	Diastereodivergent aminocatalyzed spirocyclization strategies using 4-alkylideneisoxazol-5-ones and methyl vinyl ketones. Organic Chemistry Frontiers, 2020, 7, 3599-3607.	2.3	11
1237	Elastic anisotropy, electronic and magnetic behaviours of ferromagnetic Europium Niobate EuNbO <sub>3</sub> in orthorhombic structure: DFT + U, MFA and QTAIM studies. Philosophical Magazine, 2020, 100, 2889-2911.	0.7	2
1238	Looking for the Azeotrope: A Computational Study of (Ethanol)6–Water, (Methanol)6–Water, (Ethanol)7, and (Methanol)7 Heptamers. Journal of Physical Chemistry A, 2020, 124, 7080-7087.	1.1	4
1239	Exploitation of the electron deficient outer O4 compartment of a compartmental Schiff base to act as H-bond acceptors in forming a self-assembled dimer of a manganese(III) complex: A joint experimental and theoretical venture. Polyhedron, 2020, 189, 114711.	1.0	0
1240	A theoretical insight into non-covalent supramolecular interactions in the solid state structures of two octahedral iron( <scp>iii</scp> ) complexes. CrystEngComm, 2020, 22, 5731-5742.	1.3	14
1241	Sensing mechanism elucidation of a chemosensor based on a <scp>metalâ€organic</scp> framework selective to explosive aromatic compounds. International Journal of Quantum Chemistry, 2020, 120, e26404.	1.0	14
1242	Multicomponent and multicatalytic asymmetric synthesis of furo[2,3- <i>b</i> ]pyrrole derivatives: further insights into the mode of action of chiral phosphoric acid catalysts. Chemical Science, 2020, 11, 9181-9190.	3.7	6
1243	Interactions, electronic and optical properties of nanographene–peptide complexes: a theoretical study. RSC Advances, 2020, 10, 38654-38662.	1.7	1
1244	Computer-aided design and synthesis of molecular imprinting polymers based on doubly oriented functional multiwalled carbon nanotubes for electrochemically sensing bisphenol A. Reactive and Functional Polymers, 2020, 157, 104767.	2.0	22
1245	Flat corannulene: when a transition state becomes a stable molecule. Chemical Science, 2020, 11, 13015-13025.	3.7	13
1246	Cleavage of C(sp <sup>3</sup> )–F Bonds in Trifluoromethylarenes Using a Bis(NHC)nickel(0) Complex. Journal of the American Chemical Society, 2020, 142, 19360-19367.	6.6	59
1247	Synthesis, X-ray characterization and theoretical study of 3a,6:7,9a-diepoxybenzo[de]isoquinoline derivatives: on the importance of Fâ <o 20167-20180.<="" 2020,="" 44,="" chemistry,="" interactions.="" journal="" new="" of="" td=""><td>1.4</td><td>7</td></o>	1.4	7
1248	Theoretical Characterization of the High Pressure Nonclathrate CO <sub>2</sub> Hydrate. ACS Earth and Space Chemistry, 2020, 4, 2121-2128.	1.2	1
1249	Insight Derived from Molecular Dynamics Simulation into the Selectivity Mechanism Targeting <i>c-MYC</i> G-Quadruplex. Journal of Physical Chemistry B, 2020, 124, 9773-9784.	1.2	7
1250	Oxalato bridged coordination polymer of manganese( <scp>iii</scp> ) involving unconventional Oâ⊄Ï€-hole(nitrile) and antiparallel nitrileâ⊄nitrile contacts: antiproliferative evaluation and theoretical studies. New Journal of Chemistry, 2020, 44, 20021-20038.	1.4	22
1251	Selective Activation of Aromatic Aldehydes Promoted by Dispersion Interactions: Steric and Electronic Factors of a Ĩ€â€Pocket within Cageâ€Shaped Borates for Molecular Recognition. Chemistry - A European Journal, 2020, 26, 15023-15034.	1.7	3

#	Article	IF	CITATIONS
1252	Methylene spacer regulated variation in supramolecular assembly of zinc( <scp>ii</scp> ) dicyanamide complexes with reduced Schiff base ligands: synthesis, structure and DFT study. CrystEngComm, 2020, 22, 6876-6885.	1.3	15
1253	Chiral discrimination in a mutated IDH enzymatic reaction in cancer: a computational perspective. European Biophysics Journal, 2020, 49, 549-559.	1.2	4
1254	Semicoordination Bond Breaking and Halogen Bond Making Change the Supramolecular Architecture of Metal-Containing Aggregates. Crystal Growth and Design, 2020, 20, 6956-6965.	1.4	38
1255	Computational insight into the mechanism and origin of high regioselectivity in the ring-opening cyclization of spirocyclopropanes with stabilized sulfonium ylides by the DFT. Journal of Molecular Modeling, 2020, 26, 255.	0.8	Ο
1256	Bonding Analysis of Compounds with Unusual Coordination of Carbon: Proposed Symmetric Systems with Six-Coordinate Carbon. Molecules, 2020, 25, 3937.	1.7	2
1257	Electronic and optical properties of [Au(CH <sub>3</sub> CSS)] <sub>4</sub> cluster. A quantum chemistry study. RSC Advances, 2020, 10, 33549-33557.	1.7	4
1258	The Effect of Solvent–Substrate Noncovalent Interactions on the Diastereoselectivity in the Intramolecular Carbonyl-Ene and the Staudinger [2 + 2] Cycloaddition Reactions. Journal of Physical Chemistry A, 2020, 124, 8019-8028.	1.1	5
1259	Block deformation analysis: Density matrix blocks as intramolecular deformation density. Journal of Computational Chemistry, 2020, 41, 2446-2458.	1.5	2
1260	Regiumâ^ï̃€ Bonds Are Involved in Protein–Gold Binding. Journal of Physical Chemistry Letters, 2020, 11, 8259-8263.	2.1	25
1261	Experiments and Direct Dynamics Simulations That Probe η <sup>2</sup> -Arene/Aryl Hydride Equilibria of Tungsten Benzene Complexes. Journal of the American Chemical Society, 2020, 142, 16437-16454.	6.6	13
1262	Theoretical study of the adsorption of amantadine on pristine, Al-, Ga-, P-, and As-doped boron nitride nanosheets: a PBC-DFT, NBO, and QTAIM study. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	18
1263	Metathesis of Classical and Functionalized Olefins Catalyzed by Silicaâ€Supported Singleâ€Site Wellâ€Defined W and Mo Preâ€catalysts. ChemCatChem, 2020, 12, 6067-6075.	1.8	6
1264	"Pincer―Pyridine–Dicarbene–Iridium and â€Ruthenium Complexes and Derivatives Thereof. European Journal of Inorganic Chemistry, 2020, 2020, 3359-3369.	1.0	5
1265	Steric clash in real space: biphenyl revisited. Physical Chemistry Chemical Physics, 2020, 22, 21251-21256.	1.3	16
1266	Combined DFT and MD simulation studies of protein stability on imidazolium–water (ImH <sup>+</sup> W <sub>n</sub> ) clusters with aromatic amino acids. New Journal of Chemistry, 2020, 44, 17912-17923.	1.4	6
1267	Exploring the mechanism and counterion activity regulation in the Co <sup>III</sup> (salen)-catalyzed hydration of propylene oxide. Physical Chemistry Chemical Physics, 2020, 22, 22417-22425.	1.3	5
1268	Utilizing Co-Crystallization as a Tool to Unravel the Structural Diversity and Electronic Features of I···S Halogen Bonded Interactions in Stoichiomorphic Co-Crystals. Crystal Growth and Design, 2020, 20, 6272-6282.	1.4	11
1269	Addressing the Biochemical Foundations of a Glucose-Based "Trojan Horse―Strategy to Boron Neutron Capture Therapy: From Chemical Synthesis to <i>In Vitro</i> Assessment. Molecular Pharmaceutics, 2020, 17, 3885-3899.	2.3	15

#	Article	IF	CITATIONS
1270	A theoretical review for novel Lewis base amine/imine-catalyzed reactions. Organic and Biomolecular Chemistry, 2020, 18, 6781-6800.	1.5	16
1272	A flexible bisâ€Co(III) porphyrin cage as a bimetallic catalyst for the conversion of CO <sub>2</sub> and epoxides into cyclic carbonates. ChemCatChem, 2020, 12, 5826-5833.	1.8	9
1273	Multiscale modelling investigation of wood modification with acetic anhydride. Physical Chemistry Chemical Physics, 2020, 22, 28448-28458.	1.3	13
1274	Molecular Dynamics Approach for Capturing Calixarene–Protein Interactions: The Case of Cytochrome C. Journal of Physical Chemistry B, 2020, 124, 11371-11378.	1.2	9
1275	A highly selective anthraquinone appended oxacalixarene receptor for fluorescent ICT sensing of Fâ'' ions: an experimental and computational study. Journal of Chemical Sciences, 2020, 132, 1.	0.7	13
1276	Absolute Trends and Accurate and Precise Gas-Phase Binding Energies of 1-Alkyl-3-Methylimidazolium Tetrafluoroborate Ionic Liquid Clusters from Combined Independent and Competitive TCID Measurements. Journal of Physical Chemistry A, 2020, 124, 10199-10215.	1.1	7
1277	Computational Studies of the Solid-State Molecular Organometallic (SMOM) Chemistry of Rh s-Alkane Complexes. Structure and Bonding, 2020, , 183-228.	1.0	6
1278	Halogenated Diazabutadiene Dyes: Synthesis, Structures, Supramolecular Features, and Theoretical Studies. Molecules, 2020, 25, 5013.	1.7	28
1279	A computational study on NHC-Catalyzed [3+4] annulation between isatin-derived enal and aurone-derived azadiene: Insights into mechanism and stereoselectivity. Molecular Catalysis, 2020, 496, 111183.	1.0	8
1280	Mechanistic Insights into the <i>ortho</i> -Defluorination-Hydroxylation of 2-Halophenolates Promoted by a Bis(μ-oxo)dicopper(III) Complex. Inorganic Chemistry, 2020, 59, 17018-17027.	1.9	8
1281	Cationâ^ï€ Interactions Accelerate the Living Cationic Ring-Opening Polymerization of Unsaturated 2-Alkyl-2-oxazolines. Macromolecules, 2020, 53, 3832-3846.	2.2	4
1282	The Volumetric Source Function: Looking Inside van der Waals Interactions. Scientific Reports, 2020, 10, 7816.	1.6	10
1283	Experimental distribution of electron density in crystals of Ph3Sb(O2CCH=CH–CH=CH–CH3)2 complex: the selection of a reference point for the source function in the absence of a bond critical point between atoms. Structural Chemistry, 2020, 31, 1841-1849.	1.0	1
1284	Partitioning a Molecule into the Atomic Basins and the Resultant Atomic Charges from Quantum Chemical Topology Analysis of the Kohn–Sham Potential. Journal of Physical Chemistry A, 2020, 124, 5023-5032.	1.1	3
1285	The intermolecular anthracene-transfer in a regiospecific antipodal C <sub>60</sub> difunctionalization. Organic and Biomolecular Chemistry, 2020, 18, 4090-4103.	1.5	1
1286	Tetrachloroplatinate( <scp>ii</scp> ) anion as a square-planar tecton for crystal engineering involving halogen bonding. CrystEngComm, 2020, 22, 4180-4189.	1.3	18
1287	Insights on Absolute and Relative Stereocontrol in Stereodivergent Cooperative Catalysis. Journal of the American Chemical Society, 2020, 142, 9612-9624.	6.6	29
1288	Observations of tetrel bonding between sp3-carbon and THF. Chemical Science, 2020, 11, 5289-5293.	3.7	43

ARTICLE IF CITATIONS Is breaking of a hydrogen bond enough to lead to drug resistance?. Chemical Communications, 2020, 1289 2.2 11 56, 6727-6730. Intertwined Detection and Recognition Roles of Tetrazine in Synergistic Anionâ€i€ and Hâ€bond Based 1290 1.0 Anion Receptor. ChemPhysChem, 2020, 21, 1249-1257. Quantum chemical investigation on interaction of 5-fluorouracil with cucurbiturils. Monatshefte 1291 0.9 8 Für Chemie, 2020, 151, 721-727. Understanding the first half-ALD cycle of the ZnO growth on hydroxyl functionalized carbon 1.3 nanotubes. Physical Chemistry Chémical Physics, 2020, 22, 15333-15339. Hydrogen vs. Halogen Bonds in 1-Halo-Closo-Carboranes. Materials, 2020, 13, 2163. 1293 1.310 Investigation of Cycloparaphenylenes (CPPs) and their Noncovalent Ringâ€inâ€Ring and Fullereneâ€inâ€Ring Complexes by (Matrixâ€Assisted) Laser Desorption/Ionization and Density Functional Theory. Chemistry 1294 1.7 A European Journal, 2020, 26, 8729-8741. Electron density based analysis of Nâ€"Hâ<Oî€C hydrogen bonds and electrostatic interaction energies in high-resolution secondary protein structures: insights from quantum crystallographic approaches. 1295 1.35 CrystEngComm, 2020, 22, 4363-4373. Reconciling Electrostatic and n→i€\* Orbital Contributions in Carbonyl Interactions. Angewandte 1296 7.2 Chemie - International Edition, 2020, 59, 14602-14608. Non‧ymmetrical Sterically Challenged Phenanthroline Ligands and Their Homoleptic Copper(I) 1297 1.7 19 Complexes with Improved Excited tate Properties. Chemistry - A European Journal, 2020, 26, 11887-11899. Combined Molecular Dynamics and DFT Simulation Study of the Molecular and Polymer Properties of 1298 a Catechol-Based Cyclic Oligomer of Polyether Ether Ketone. Polymers, 2020, 12, 1054. "Antiâ€elektrostatische―Halogenbrücken. Angewandte Chemie, 2020, 132, 11244-11251. 1299 10 1.6 Anion Binding Affinity: Acidity versus Conformational Effects. Journal of Organic Chemistry, 2020, 85, 8074-8084. NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102. 1301 1.2 425 Symmetrical Noncovalent Interactions Br·Â·À·Br Observed in Crystal Structure of Exotic Primary 1.1 Peroxide. Symmetry, 2020, 12, 637. Comparative investigation of  $\hat{A}\pm \hat{I}f\hat{a}\in$  hole interactions of carbon-containing molecules with Lewis bases, 1303 1.0 18 acids and di-halogens. Chemical Papers, 2020, 74, 3569-3580. QM/MM-MD dissociation of Ag+ and H+ mediated cytosine pairs: Monomers and dimers. Journal of 1304 Örganometallic Chemistry, 2020, 919, 121333. Mixed micellization of bile salts and transglycosylated stevia and enhanced binding and solubility of 1305 non-steroidal anti-inflammatory drugs using mixed micelle. Journal of Molecular Liquids, 2020, 311, 2.312 113341. NCIPLOT4: Fast, Robust, and Quantitative Analysis of Noncovalent Interactions. Journal of Chemical 2.3 Theory and Computation, 2020, 16, 4150-4158.

#	Article	IF	CITATIONS
1307	Quantifying Intramolecular Halogen Bonds in Nucleic Acids: A Combined Protein Data Bank and Theoretical Study. ACS Chemical Biology, 2020, 15, 1942-1948.	1.6	18
1308	C–H Amination Mediated by Cobalt Organoazide Adducts and the Corresponding Cobalt Nitrenoid Intermediates. Journal of the American Chemical Society, 2020, 142, 11232-11243.	6.6	44
1309	A detailed look at the bonding interactions in the microsolvation of monoatomic cations. Physical Chemistry Chemical Physics, 2020, 22, 13049-13061.	1.3	20
1310	Molecular dynamics study of functionally relevant interdomain and active site interactions in the autotransporter esterase EstA from <i>Pseudomonas aeruginosa</i> . Molecular Simulation, 2020, 46, 743-756.	0.9	0
1311	A theoretical perspective of the agostic effect in early transition metal compounds. Coordination Chemistry Reviews, 2020, 419, 213401.	9.5	32
1312	Two copper (II) complexes derived from anthranilic acid and 4-iodo-anthranilic acid Schiff bases: Structural elucidation, halogen bonding interactions and catalytic study using 3,5-DTBC. Journal of Molecular Structure, 2020, 1217, 128398.	1.8	7
1313	Selective Halogenation of Pyridines Using Designed Phosphine Reagents. Journal of the American Chemical Society, 2020, 142, 11295-11305.	6.6	39
1314	Sulfur hydrogen bonding and internal dynamics in the monohydrates of thenyl mercaptan and thenyl alcohol. Physical Chemistry Chemical Physics, 2020, 22, 12412-12421.	1.3	21
1315	Multiconfigurational dynamics explain photochemical reactivity and torquoselectivity towards fluorinated polyacetylenes. Journal of Materials Chemistry C, 2020, 8, 10880-10888.	2.7	2
1316	Growth Pattern, Stability, and Properties of Complexes of C <sub>2</sub> H <sub>5</sub> OH and <i>n</i> CO <sub>2</sub> ( <i>n</i> = 1–5) Molecules: A Theoretical Study. ACS Omega, 2020, 5, 14408-14416.	1.6	2
1317	Size dependent hydrogen-bonded methanol wires regulating the fluorescence On-Off of 1-H-pyrrolo[3,2-h]quinoline·(MeOH)n=1,2 complexes with ESMPT. Journal of Molecular Liquids, 2020, 306, 112894.	2.3	14
1318	Components of the interaction energy of the odd-electron halogen bond: an <i>ab initio</i> study. Physical Chemistry Chemical Physics, 2020, 22, 15389-15400.	1.3	6
1319	Tribute to David N. Beratan. Journal of Physical Chemistry B, 2020, 124, 3437-3440.	1.2	0
1320	In Silico Design of Cylindrophanes: The Role of Functional Groups in a Fluoride Selective Host. ChemPhysChem, 2020, 21, 1989-2005.	1.0	5
1321	Zigzag vs Helicoidal Gold–Silver 1D Chains: Influence of Subtle Interactions in the Spatial Arrangement of Supramolecular Systems. Inorganic Chemistry, 2020, 59, 9443-9451.	1.9	2
1322	W2SDD theory for computational thermochemistry: study of the addition of hydrogen halide to propene. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	8
1323	Azafluorene derivatives as inhibitors of SARS CoV-2 RdRp: Synthesis, physicochemical, quantum chemical, modeling and molecular docking analysis. Journal of Molecular Structure, 2020, 1220, 128741.	1.8	28
1324	Halogen Bonds in Protein Nucleic Acid Recognition. Journal of Chemical Theory and Computation, 2020, 16, 4744-4752.	2.3	25

#	Article	IF	CITATIONS
1325	Hydrogen bond interactions of hydrated aluminum nitrate with <scp>PVDF</scp> , <scp>PVDFâ€TrFE,</scp> and <scp>PVDFâ€HFP</scp> : A density functional theoryâ€based illustration. International Journal of Quantum Chemistry, 2020, 120, e26328.	1.0	13
1326	Microhydration of protonated biomolecular building blocks: protonated pyrimidine. Physical Chemistry Chemical Physics, 2020, 22, 13092-13107.	1.3	7
1327	A semipinacol rearrangement of vinylogous α-ketol cocatalyzed by a cinchona-based primary amine and N-Boc-phenylglycines: mechanisms, roles of catalysts and the origin of enantioselectivity. Organic Chemistry Frontiers, 2020, 7, 1845-1861.	2.3	6
1328	Structural Characterization, DFT Calculation, NCI, Scan-Rate Analysis and Antifungal Activity against Botrytis cinerea of (E)-2-{[(2-Aminopyridin-2-yl)imino]-methyl}-4,6-di-tert-butylphenol (Pyridine Schiff) Tj ETQq1 1	01784314	⊦rgBT /Overl
1329	Engineering Crystals Using sp 3   Centred Tetrel Bonding Interactions. Chemistry - A European Journal, 2020, 26, 10126-10132.	1.7	28
1330	High sensitivity of graphdiyne nanoflake toward detection of phosgene, thiophosgene and phosogenoxime; a first-principles study. Journal of Molecular Graphics and Modelling, 2020, 100, 107658.	1.3	45
1331	Density-functional study of hydrazine doped single-walled carbon nanotubes as an n-type semiconductor. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 124, 114306.	1.3	3
1332	Directing the Crystal Packing in Triphenylphosphine Gold(I) Thiolates by Ligand Fluorination. Inorganic Chemistry, 2020, 59, 8667-8677.	1.9	13
1333	Diversity and uniformity in anionâ€"ï€ complexes of thiocyanate with aromatic, olefinic and quinoidal ï€-acceptors. Dalton Transactions, 2020, 49, 8734-8743.	1.6	19
1334	Reconciling Electrostatic and n→ï€* Orbital Contributions in Carbonyl Interactions. Angewandte Chemie, 2020, 132, 14710-14716.	1.6	8
1335	Improving the picture of atomic structure in nonoriented polymer domains using the pair distribution function: A study of polyamide 6. Journal of Polymer Science, 2020, 58, 1843-1866.	2.0	6
1336	Gas Phase Computational Study of Diclofenac Adsorption on Chitosan Materials. Molecules, 2020, 25, 2549.	1.7	3
1337	Crystal structure and homopolar dihydrogen interactions in propanoâ€bridged indigo. Journal of Physical Organic Chemistry, 2020, 33, e4096.	0.9	3
1338	Arene vs. Alkene Substrates in Ruâ€Catalyzed Olefin Metathesis: a DFT Investigation. European Journal of Organic Chemistry, 2020, 2020, 4743-4749.	1.2	5
1339	Computational Insight into the Mechanism of Mannich Reaction between Glycinate and Aryl <i>N</i> â€Diphenylphosphinyl Imine Catalyzed by Nâ€Quaternized Pyridoxal. ChemistrySelect, 2020, 5, 6504-6513.	0.7	3
1340	π-Hole··· <i>d</i> <sub><i>z</i></sub> <sup>2</sup> [Pt <sup>II</sup> ] Interactions with Electron-Deficient Arenes Enhance the Phosphorescence of Pt <sup>II</sup> -Based Luminophores. Inorganic Chemistry, 2020, 59, 9308-9314.	1.9	39
1341	Analysis of crystal field effects and interactions using X-ray restrained ELMOs. Journal of Molecular Structure, 2020, 1209, 127975.	1.8	21
1342	Asymmetric [N–l–N] <sup>+</sup> halonium complexes. Chemical Communications, 2020, 56, 8428-8431.	2.2	41

#	Article	IF	CITATIONS
1343	Principal interacting orbital: A chemically intuitive method for deciphering bonding interaction. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1469.	6.2	67
1344	Energetics of Dynamic Kinetic Asymmetric Transformation in Suzuki–Miyaura Coupling. ACS Catalysis, 2020, 10, 4349-4360.	5.5	6
1345	Enantioselective Allenoate-Claisen Rearrangement Using Chiral Phosphate Catalysts. Journal of the American Chemical Society, 2020, 142, 6390-6399.	6.6	50
1346	Synthesis, X-ray characterization and regium bonding interactions of a trichlorido(1-hexylcytosine)gold( <scp>iii</scp> ) complex. Chemical Communications, 2020, 56, 3524-3527.	2.2	28
1347	Unraveling the Elastic Properties of (Quasi)Two-Dimensional Hybrid Perovskites: A Joint Experimental and Theoretical Study. ACS Applied Materials & Interfaces, 2020, 12, 17881-17892.	4.0	21
1348	Evaluation the synergistic antitumor effect of methotrexate–camptothecin codelivery prodrug from selfâ€assembly process to acidâ€catalyzed both drugs release: A comprehensive theoretical study. Journal of Computational Chemistry, 2020, 41, 1486-1496.	1.5	11
1349	Octapodal Corannulene Porphyrin-Based Assemblies: Allosteric Behavior in Fullerene Hosting. Journal of Organic Chemistry, 2020, 85, 4918-4926.	1.7	14
1350	Computational Analysis of the Selective Formation of the C4α—C8′ Bond in the Intermolecular Coupling of Catechin Derivatives. Journal of Organic Chemistry, 2020, 85, 5010-5018.	1.7	2
1351	Unveiling the Impact of Aggregation on Optical Anisotropy of Triazaacephenanthrylene Single Crystals. A Combined Quantum Crystallography and Conceptual Density Functional Theory Approach. Journal of Physical Chemistry A, 2020, 124, 2931-2941.	1.1	4
1352	The Aromatic 2-Iminomethylphenyltellurenyl Cation. A Lewis Superacid Despite the Intramolecularly Coordinating N-Donor Ligand. Organometallics, 2020, 39, 1202-1212.	1.1	10
1353	Expanding the horizons of covalent organic frameworks to electrochemical sensors; A case study of CTF-FUM. Microporous and Mesoporous Materials, 2020, 300, 110146.	2.2	30
1354	Supramolecular lead( <scp>ii</scp> ) architectures engineered by tetrel bonds. CrystEngComm, 2020, 22, 2389-2396.	1.3	29
1355	Rotational spectrum and intramolecular hydrogen bonding in 1,2-butanedithiol. Journal of Molecular Structure, 2020, 1211, 128080.	1.8	8
1356	Halogen Bonding Provides Heterooctameric Supramolecular Aggregation of Diaryliodonium Thiocyanate. Crystals, 2020, 10, 230.	1.0	25
1357	AgN <sub>3</sub> -Catalyzed Hydroazidation of Terminal Alkynes and Mechanistic Studies. Journal of the American Chemical Society, 2020, 142, 7083-7091.	6.6	19
1358	Complexity Reduction in Density Functional Theory Calculations of Large Systems: System Partitioning and Fragment Embedding. Journal of Chemical Theory and Computation, 2020, 16, 2952-2964.	2.3	19
1359	Supramolecular and theoretical perspectives of 2,2′:6′,2′′-terpyridine based Ni( <scp>ii</scp> ) and Cu( <scp>ii</scp> ) complexes: on the importance of C–H⋯Cl and π⋯I€ interactions. New Journal of Chemistry, 2020, 44, 7310-7318.	1.4	22
1360	Non-covalent interactions with inverted carbon: a carbo-hydrogen bond or a new type of hydrogen bond?. Physical Chemistry Chemical Physics, 2020, 22, 8988-8997.	1.3	21

	CITATION REF	ORT	
#	Article	IF	CITATIONS
1361	"Antiâ€Electrostatic―Halogen Bonding. Angewandte Chemie - International Edition, 2020, 59, 11150-11157.	7.2	59
1362	Structural motifs of oxacalix[4]arene for molecular recognition of nitroaromatic explosives: Experimental and computational investigations of host-guest complexes. Journal of Molecular Liquids, 2020, 306, 112809.	2.3	21
1363	Charge-assisted hydrogen bond and nitrileâ< nitrile interaction directed supramolecular associations in Cu( <scp>ii</scp> ) and Mn( <scp>ii</scp> ) coordination complexes: anticancer, hematotoxicity and theoretical studies. New Journal of Chemistry, 2020, 44, 5473-5488.	1.4	34
1364	Azaphenantherene derivatives as inhibitor of SARS CoV-2 Mpro: Synthesis, physicochemical, quantum chemical and molecular docking analysis. Chemical Data Collections, 2020, 28, 100470.	1.1	2
1365	Adipato bridged novel hexanuclear Cu( <scp>ii</scp> ) and polymeric Co( <scp>ii</scp> ) coordination compounds involving cooperative supramolecular assemblies and encapsulated guest water clusters in a square grid host: antiproliferative evaluation and theoretical studies. Dalton Transactions, 2020, 49, 9863-9881.	1.6	27
1366	MOF Encapsulation of Ru Olefin Metathesis Catalysts to Block Catalyst Decomposition. Catalysts, 2020, 10, 687.	1.6	9
1367	A molecular electron density theory study of the [3 + 2] cycloaddition reaction of 1,4-diphosphorinium-3-olates with methyl acrylate and methyl methacrylate. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	1
1368	Engineering Electrical Conductivity in Stable Zirconium-Based PCN-222 MOFs with Permanent Mesoporosity. Chemistry of Materials, 2020, 32, 6137-6149.	3.2	34
1369	Non-covalent interactions between sertraline stereoisomers and 2-hydroxypropyl-β-cyclodextrin: a quantum chemistry analysis. RSC Advances, 2020, 10, 20202-20210.	1.7	6
1371	Theoretical Study of the Structures of 4-(2,3,5,6-Tetrafluoropyridyl)Diphenylphosphine Oxide and Tris(Pentafluorophenyl)Phosphine Oxide: Why Does the Crystal Structure of (Tetrafluoropyridyl)Diphenylphosphine Oxide Have Two Different P=O Bond Lengths?. Molecules, 2020, 25. 2778.	1.7	0
1372	Aldehyde trapping by self-propagating atom-exchange reactions on a gallium nitride monolayer: role of the molecule complexity. New Journal of Chemistry, 2020, 44, 12843-12849.	1.4	6
1373	Making Base-Assisted C–H Bond Activation by Cp*Co(III) Effective: A Noncovalent Interaction-Inclusive Theoretical Insight and Experimental Validation. Organometallics, 2020, 39, 2609-2629.	1.1	13
1374	The definitive challenge of forming uncommon pseudoâ€i€Â·Â·Ĥa€"F and C···Ha€"F hydrogen bonds on cycli and cubic nonpolar hydrocarbons. Journal of Physical Organic Chemistry, 2020, 33, e4098.	с <sub>0.9</sub>	0
1375	Characterization and Decomposition of the Natural van der Waals SnSb <sub>2</sub> Te <sub>4</sub> under Compression. Inorganic Chemistry, 2020, 59, 9900-9918.	1.9	31
1376	Regio- and stereochemistry in the aza-Diels–Alder reaction of an azoalkene with furan and 2,3-dihydrofuran: a molecular electron density theory study. Structural Chemistry, 2020, 31, 2161-2170.	1.0	6
1377	Unravelling the regio- and stereoselective synthesis of bicyclic N,O-nucleoside analogues within the molecular electron density theory perspective. Structural Chemistry, 2020, 31, 2147-2160.	1.0	13
1378	Quantitative assessment of intramolecular hydrogen bonds in neutral histidine. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	20
1379	The Affinity of Some Lewis Bases for Hexafluoroisopropanol as a Reference Lewis Acid: An ITC/DFT Study. ChemPhysChem, 2020, 21, 2136-2142.	1.0	7

ARTICLE IF CITATIONS Investigating greenhouse gas adsorption in MOFs SIFSIX-2-Cu, SIFSIX-2-Cu-i, and SIFSIX-3-Cu through 1380 0.8 7 computational studies. Journal of Molecular Modeling, 2020, 26, 188. Halogenation of the N â€Terminus Tyrosine 10 Promotes Supramolecular Stabilization of the Amyloidâ€Ĵ² Sequence 7–12. ChemistryOpen, 2020, 9, 253-260. Tuning of interactions between cathode and lithium polysulfide in Li-S battery by rational 1382 19 7.1 halogenation. Journal of Energy Chemistry, 2020, 49, 147-152. Hydrogen bond capability tunable different "relay-race―mechanisms of the excited-state proton 1.4 transfer process for 4â€2-methoxy-3-hydroxyflavone. Organic Electronics, 2020, 81, 105678. Chiral phosphoric acid catalyzed asymmetric arylation of indoles<i>via</i>nucleophilic aromatic substitution: mechanisms and origin of enantioselectivity. Catalysis Science and Technology, 2020, 10, 1384 2.1 9 2277-2292. Novel <i>cis</i>-[PdCl<sub>2</sub>(NHC)(PPh<sub>3</sub>)] complex: synthesis, crystal structure, spectral investigations, DFT and NCI studies, prediction of biological activity. Journal of Coordination 0.8 Chemistry, 2020, 73, 525-543. Capturing the Monomeric (L)CuH in NHCâ€Capped Cyclodextrin: Cavityâ€Controlled Chemoselective 1386 1.6 13 Hydrosilylation of  $\hat{1}\pm,\hat{l}^2\hat{a}\in$ Unsaturated Ketones. Angewandte Chemie, 2020, 132, 7661-7667. Capturing the Monomeric (L)CuH in NHCâ€Capped Cyclodextrin: Cavityâ€Controlled Chemoselective Hydrosilylation of î±,î²â€Unsaturated Ketones. Angewandte Chemie - International Edition, 2020, 59, 7.2 44 7591-7597. Unconventional DNA-relevant π-stacked hydrogen bonded arrays involving supramolecular guest benzoate dimers and cooperative anionâ€"΀/Ï€â€"î€/Ï€â€"anion contacts in coordination compounds of 1388 1.4 24 Co(<scp>ii</scp>) and Zn(<scp>ii</scp>) phenanthroline: experimental and theoretical studies. New Journal of Chemistry, 2020, 44, 4504-4518 Amino acid ionic liquids as potential candidates for CO2 capture: Combined density functional theory 1389 1.2 and molecular dynamics simulations. Chemical Physics Letters, 2020, 745, 137239. Cyclic versus straight chain oligofuran as sensor: A detailed DFT study. Journal of Molecular 1390 1.3 66 Graphics and Modelling, 2020, 97, 107569. Vanadyl Species Catalyzed 1,2-Oxidative Trifluoromethylation of Unactivated Olefins. ACS Catalysis, 5.5 2020, 10, 3676-3683. Mechanistic Study on Ag<sup>I</sup>-Catalyzed Oxidative Cross-Coupling/Cyclization between Terminal Alkynes and Î<sup>2</sup>-Enamino Esters under Base Conditions. Journal of Organic Chemistry, 2020, 85, 1392 1.7 5 4408-4417. Theoretical investigation of intermolecular hydrogen bond induces fluorescence quenching 1393 1.5 23 phenomenon for Coumarin-1. Journal of Luminescence, 2020, 221, 117110. Theoretical study on the relationship between the position of the substituent and the ESIPT 1394 0.7 11 fluorescence characteristic of HPIP\*. Chinese Physics B, 2020, 29, 038201. Skillfully tuning 1-hydroxy-9H-fluoren-9-one forward-backward ESIPT processes by introducing 1395 electron-withdrawing groups: A theoretical exploration. Journal of Molecular Liquids, 2020, 303, 2.3 39 112627. Onâ€Surface Assembly of Hydrogen―and Halogenâ€Bonded Supramolecular Graphyneâ€Like Networks. 1396 1.6 3 Angewandte Chemie, 2020, 132, 9636-9642. Onâ€Surface Assembly of Hydrogen†and Halogenâ€Bonded Supramolecular Graphyneâ€Like Networks. Angewandte Chemie - International Edition, 2020, 59, 9549-9555.

#	Article	IF	CITATIONS
1398	Theoretical investigation on the ESIPT mechanism and fluorescent sensing mechanism of 2-(2′-hydroxyphenyl) thiazole-4-carboxaldeyde in methanol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 233, 118214.	2.0	19
1399	New Way for Probing Bond Strength. Journal of Physical Chemistry A, 2020, 124, 1850-1860.	1.1	121
1400	Nickel-catalysed anti-Markovnikov hydroarylation of unactivated alkenes with unactivated arenes facilitated by non-covalent interactions. Nature Chemistry, 2020, 12, 276-283.	6.6	129
1401	A combined experimental and theoretical study on an ionic cobalt(III/II) complex with a Schiff base ligand. Polyhedron, 2020, 182, 114432.	1.0	5
1402	Aromaticity as a Guide to Planarity in Conjugated Molecules and Polymers. Journal of Physical Chemistry C, 2020, 124, 5608-5612.	1.5	11
1403	Competition and cooperativity of hydrogen-bonding and tetrel-bonding interactions involving triethylene diamine (DABCO), H <sub>2</sub> O and CO <sub>2</sub> in air. New Journal of Chemistry, 2020, 44, 2328-2338.	1.4	25
1404	Synthesis, X-ray Characterization and Density Functional Theory (DFT) Studies of Two Polymorphs of the α,α,α,α, Isomer of Tetra-p-Iodophenyl Tetramethyl Calix[4]pyrrole: On the Importance of Halogen Bonds. Molecules, 2020, 25, 285.	1.7	3
1405	DFT/TD-DFT study on development and optimization of 1- anilino-3-phenyliminourea as a colorimetric chemosensor for Hg2+ recognition in aqueous medium. Journal of Molecular Structure, 2020, 1206, 127699.	1.8	11
1406	Formation of Formic Acid Derivatives through Activation and Hydroboration of CO <sub>2</sub> by Low-Valent Group 14 (Si, Ge, Sn, Pb) Catalysts. Journal of Physical Chemistry A, 2020, 124, 1121-1133.	1.1	18
1407	Feasibility of pristine, Al-doped and Ga-doped Boron Nitride nanotubes for detecting SF4 gas: A DFT, NBO and QTAIM investigation. Applied Surface Science, 2020, 510, 145490.	3.1	63
1408	Theoretical study of glycine amino acid adsorption on graphene oxide. Journal of Molecular Modeling, 2020, 26, 33.	0.8	8
1409	Are Anions of Cyclobutane Beryllium Derivatives Stabilized through Four-Center One-Electron Bonds?. Journal of Physical Chemistry A, 2020, 124, 1515-1521.	1.1	3
1410	A series of hydrogen bond mediated dinuclear nickel(II) complexes with reduced Schiff base ligands: An insight into the nature of their short intermolecular hydrogen bonds. Polyhedron, 2020, 179, 114374.	1.0	13
1411	Protonation of Naphthalene–(Water) <sub><i>n</i></sub> Nanoclusters: Intracluster Proton Transfer to Hydration Shell Revealed by Infrared Photodissociation Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 1134-1151.	1.1	20
1412	Simple iodoalkyne-based organocatalysts for the activation of carbonyl compounds. Organic and Biomolecular Chemistry, 2020, 18, 1594-1601.	1.5	19
1413	Asymmetric Synthesis of Axially Chiral Phosphamides via Atroposelective <i>N</i> -Allylic Alkylation. ACS Catalysis, 2020, 10, 2324-2333.	5.5	50
1414	A newly synthesized nitrogenâ€rich derivative of bicyclic quinoxaline—Structural and conceptual DFT reactivity study. Journal of Physical Organic Chemistry, 2020, 33, e4055.	0.9	19
1415	Insight into the factors controlling the equilibrium of allylic azides. RSC Advances, 2020, 10, 4404-4413.	1.7	7

#	Article	IF	CITATIONS
1416	Metal–Organic Frameworks of Cu(II) Constructed from Functionalized Ligands for High Capacity H <sub>2</sub> and CO <sub>2</sub> Gas Adsorption and Catalytic Studies. Inorganic Chemistry, 2020, 59, 1810-1822.	1.9	25
1417	Chargeâ€Assisted Chalcogen Bonds: CSD and DFT Analyses and Biological Implication in Glucosidase Inhibitors. Chemistry - A European Journal, 2020, 26, 4599-4606.	1.7	42
1418	Clamâ€like Cyclotricatechyleneâ€based Capsules: Identifying the Roles of Protonation State and Guests as well as the Drivers for Stability and (Antiâ€)Cooperativity. Chemistry - an Asian Journal, 2020, 15, 1301-1314.	1.7	4
1419	Lignin solvation by ionic liquids: The role of cation. Journal of Molecular Liquids, 2020, 303, 112588.	2.3	17
1420	Crystal Structures of Dimethoxyanthracens: A Clue to a Rational Design of Packing Structures of π onjugated Molecules. Chemistry - an Asian Journal, 2020, 15, 915-919.	1.7	10
1421	A rotational study of the AlaAla dipeptide. Physical Chemistry Chemical Physics, 2020, 22, 13867-13871.	1.3	10
1422	Revealing the Interplay Between Covalent and Non-Covalent Interactions Driving the Adsorption of Monosubstituted Thiourea Derivatives on the Au(111) Surface. Journal of Physical Chemistry C, 2020, 124, 9924-9939.	1.5	2
1423	Structural, Non-Covalent Interaction, and Natural Bond Orbital Studies on Bromido-Tricarbonyl Rhenium(I) Complexes Bearing Alkyl-Substituted 1,4-Diazabutadiene (DAB) Ligands. Crystals, 2020, 10, 267.	1.0	6
1424	New metal chelate constructed from Ni(NCS)2 and 1,2-diphenyl-1,2-bis((phenyl(pyridin-2-yl)methylene)hydrazono)ethane. Inorganica Chimica Acta, 2020, 509, 119707.	1.2	7
1425	Potential of Mean Force Calculations for an S <sub>N</sub> 2 Fluorination Reaction in Five Different Imidazolium Ionic Liquid Solvents Using Quantum Mechanics/Molecular Mechanics Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 4338-4357.	1.2	9
1426	High-performance carbon dioxide capture and storage by multi-functional sphingosine kinase inhibitors through a CO <sub>2</sub> -philic membrane. New Journal of Chemistry, 2020, 44, 7771-7779.	1.4	10
1427	Solid-state fluorescent 1,2,4-triazole zinc(II) complexes: Self-organization via bifurcated (N H)2â⊄Cl contacts. Inorganica Chimica Acta, 2020, 510, 119660.	1.2	3
1428	Encapsulation of Mg <sub>2</sub> inside a C <sub>60</sub> cage forms an electride. Journal of Computational Chemistry, 2020, 41, 1645-1653.	1.5	20
1429	Understanding the mechanism of [3 + 2] cycloaddition reaction of benzoisothiazole-2,2-dioxide-3-ylidene with nitrones. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	1
1430	Modulating ESIPT behavior and fluorescent sensing mechanism of 2-(2′-hydroxyphenol)thiazole-4-carbonxaldeyde derivatives: A theoretical study. Chemical Physics Letters, 2020, 747, 137342.	1.2	3
1431	Synthesis of thiosemicarbazone-based colorimetric chemosensor for Cu2+ ions' recognition in aqueous medium: Experimental and theoretical studies. Journal of Molecular Structure, 2020, 1212, 128094.	1.8	11
1432	Unravelling the kinetics and molecular mechanism of the degenerate Cope rearrangement of bullvalene. New Journal of Chemistry, 2020, 44, 6543-6552.	1.4	8
1433	A molecular electron density theory study to understand the interplay of theory and experiment in nitrone-enone cycloaddition. Journal of Chemical Sciences, 2020, 132, 1.	0.7	13

#	Article	IF	CITATIONS
1434	Exotic Two-Dimensional Structure: The First Case of Hexagonal NaCl. Journal of Physical Chemistry Letters, 2020, 11, 3821-3827.	2.1	38
1435	Supramolecular Assembly of Thiopheneâ€Based Oligomers into Nanostructured Fluorescent Conductive and Chiral Microfibers. ChemistryOpen, 2020, 9, 499-511.	0.9	4
1436	Protic vs aprotic ionic liquid for CO2 fixation: A simulation study. Green Energy and Environment, 2020, 5, 183-194.	4.7	49
1437	Non-covalent interactions induced supramolecular architecture of Hg(NCS)2 with 3-pyridinecarbaldehyde nicotinoylhydrazone. Inorganica Chimica Acta, 2020, 509, 119700.	1.2	9
1438	Computational design of an intramolecular frustrated lewis pair catalyst for enantioselective hydrogenation. Journal of Theoretical and Computational Chemistry, 2020, 19, 2050009.	1.8	0
1439	Development of P- and N-Chirogenic Ligands Based on Chiral Induction from a Phosphorus Donor to a Nitrogen Donor in Palladium Complexes. Organometallics, 2020, 39, 1672-1677.	1.1	5
1440	Control over Kinetic and Thermodynamically Driven Pathways of Crystallization to Yield Cofacial and Slipped‣tack Dimers in Single Crystals. Chemistry - A European Journal, 2020, 26, 10501-10509.	1.7	10
1441	The Ï€â€hole tetrel bond between <scp>X<sub>2</sub>TO</scp> and <scp>CO<sub>2</sub></scp> : Substituent effects and its potential adsorptivity for <scp>CO<sub>2</sub></scp> . International Journal of Quantum Chemistry, 2020, 120, e26251.	1.0	15
1442	Methylone screening with electropolymerized molecularly imprinted polymer on screen-printed electrodes. Sensors and Actuators B: Chemical, 2020, 316, 128133.	4.0	23
1443	Mechanistic details of metalâ€free cyclization reaction of organophosphorus oxide with alkynes mediated by 2,6″utidine and Tf 2 O. Journal of Computational Chemistry, 2020, 41, 1709-1717.	1.5	5
1444	Tuning of the Coordination and Emission Properties of 4-Amino-2,1,3-Benzothiadiazole by Introduction of Diphenylphosphine Group. Crystal Growth and Design, 2020, 20, 5796-5807.	1.4	22
1445	Computational insight into the halogen bonded self-assembly of hexa-coordinated metalloporphyrins. Physical Chemistry Chemical Physics, 2020, 22, 11558-11566.	1.3	13
1446	Neutral binary chalcogen–nitrogen and ternary S,N,P molecules: new structures, bonding insights and potential applications. Dalton Transactions, 2020, 49, 6532-6547.	1.6	8
1447	Soft X-ray Absorption Spectroscopy Probes OH··Â-Ï€ Interactions in Epoxy-Based Polymers. Journal of Physical Chemistry C, 2020, 124, 9622-9627.	1.5	9
1448	Zinc(II) complexes derived from 2-formylpyridine nicotinoyl hydrazone as organic blocker: Syntheses, crystal architectures, Hirshfeld surface analyses and DFT studies. Journal of Molecular Structure, 2021, 1229, 129614.	1.8	1
1449	Elastic isotropy, magnetic and electronic properties, bonding and non-covalent interactions analyses of HoFe4P12 filled-skutterudite: DFTÂ+ÂUÂ+ÂSOC, QTAIM and NCI investigations. Journal of Magnetism and Magnetic Materials, 2021, 518, 167435.	1.0	4
1450	Structure-property correlation in gallic acid and 4-cyanopyridine cocrystal and binding studies with drug efflux pump in bacteria. Journal of Molecular Structure, 2021, 1225, 129279.	1.8	4
1451	Analysis of supramolecular interactions directing crystal packing of a A combination of XRD, MEP, NBO, QTAIM, and NCI analyses. Journal of Molecular Structure, 2021, 1228, 129438.	1.8	3

#	Article	IF	CITATIONS
1452	Shedding light on the factors controlling the mechanism, selectivity and reactivity of the Diels–Alder reactions between substituted pyridinones and ethylenes: a MEDT study. Molecular Physics, 2021, 119, e1828635.	0.8	4
1453	The adsorption of bromochlorodifluoromethane on pristine and Ge-doped silicon carbide nanotube: a PBC-DFT, NBO, and QTAIM study. Structural Chemistry, 2021, 32, 481-494.	1.0	27
1454	Binding of SARS oVâ€2 to Cell Receptors: A Tale of Molecular Evolution. ChemBioChem, 2021, 22, 724-732.	1.3	27
1455	MEDT study of the 1,3-DC reaction of diazomethane with Psilostachyin and investigation about the interactions of some pyrazoline derivatives with protease (Mpro) of nCoV-2. Journal of Molecular Graphics and Modelling, 2021, 102, 107763.	1.3	20
1456	The adsorption of bromochlorodifluoromethane on pristine, Al, Ga, P, and As-doped boron nitride nanotubes: A study involving PBC-DFT, NBO analysis, and QTAIM. Computational and Theoretical Chemistry, 2021, 1193, 113047.	1.1	22
1457	Noncovalent functionalization of graphene through physisorption of 1,1-diamino-2,2-dinitroethene: Impacts of and cooperativity between hydrogen bond and π···π interaction. Journal of Physics and Chemistry of Solids, 2021, 148, 109736.	1.9	4
1458	Synthesis, X-ray characterization, Hirshfeld surface analysis and DFT calculations on tetrazolyl-phenol derivatives: H-bonds vs C–H…π/π…π interactions. Journal of Molecular Structure, 2021, 1227, 129425.	1.8	9
1459	Pyridoxal derived AlEgen as a fluorescent pH sensor. Dyes and Pigments, 2021, 184, 108844.	2.0	35
1460	The Keto–Enol Tautomerism of Biliverdin in Bacteriophytochrome: Could it Explain the Bathochromic Shift in the Pfr Form? â€. Photochemistry and Photobiology, 2021, 97, 99-109.	1.3	2
1461	The Sizeâ€Accelerated Kinetic Resolution of Secondary Alcohols. Angewandte Chemie - International Edition, 2021, 60, 774-778.	7.2	17
1462	Fractionation of lignin using organic solvents: A combined experimental and theoretical study. International Journal of Biological Macromolecules, 2021, 168, 792-805.	3.6	39
1463	Impact of Organic Templates on the Selective Formation of Zeolite Oligomers. Angewandte Chemie - International Edition, 2021, 60, 7111-7116.	7.2	7
1464	Impact of Organic Templates on the Selective Formation of Zeolite Oligomers. Angewandte Chemie, 2021, 133, 7187-7192.	1.6	9
1465	Supramolecular association and quantification of intermolecular interactions of 4′-functionalized 2,2′:6′,2″-terpyridines: Experimental observation and theoretical studies. Journal of Molecular Structure, 2021, 1226, 129254.	1.8	11
1466	Theoretical study of chloride complexes with hybrid macrocycles. New Journal of Chemistry, 2021, 45, 463-470.	1.4	1
1467	Possible Mechanisms and Origin of Selectivities for Phosphineâ€Catalyzed [2+n] (n=3, 4) Annulations of Saturated Amines and Î′â€Acetoxy Allenoates. Asian Journal of Organic Chemistry, 2021, 10, 619-625.	1.3	10
1468	Role of fluorine-fluorine and weak intermolecular interactions in the supramolecular network of a new trifluoromethyl-1,5-benzodiazepine: Crystal structure, Hirshfeld surface analysis and theoretical study. Journal of Fluorine Chemistry, 2021, 242, 109697.	0.9	9
1469	Substituent effects on the photophysical properties of 2,9â€substituted phenanthroline copper(I) complexes: a theoretical investigation. ChemPhysChem, 2021, 22, 509-515.	1.0	7

#	ARTICLE Construction of Helical Structures with Multiple Fused Anthracenes: Structures and Properties of	IF 1.7	CITATIONS
1470	Long Expanded Helicenes. Chemistry - A European Journal, 2021, 27, 4548-4552. Heteroleptic Zn(II) 3,5-diiodosalicylates: Structures, luminescence and features of non-covalent interactions in solid state. Polyhedron, 2021, 194, 114895.	1.7	10
1472	London Dispersion Interactions Rather than Steric Hindrance Determine the Enantioselectivity of the Corey–Bakshi–Shibata Reduction. Angewandte Chemie - International Edition, 2021, 60, 4823-4832.	7.2	57
1473	Bifurcated μ< <sub>2</sub> -l···(N,O) Halogen Bonding: The Case of (Nitrosoguanidinate)Ni <sup>II</sup> Cocrystals with Iodine(I)-Based Ĭƒ-Hole Donors. Crystal Growth and Design, 2021, 21, 588-596.	1.4	24
1474	An Ultimate Investigation on the Adsorption of Amantadine on Pristine and Decorated Fullerenes C59X (X=Si, Ge, B, Al, Ga, N, P, and As): A DFT, NBO, and QTAIM Study. Journal of Computational Biophysics and Chemistry, 2021, 20, 23-39.	1.0	28
1475	Iron-catalysed asymmetric carboazidation of styrenes. Nature Catalysis, 2021, 4, 28-35.	16.1	60
1476	A first exploration of isostructurality in transition metal nitroprussides: X-ray analysis, magnetic properties and DFT calculations. CrystEngComm, 2021, 23, 1158-1171.	1.3	3
1477	Ligand structure-driven self-assembly of Zn(NCS)2 with a carbohydrazone ligand: A possible intermediate towards a [2Â×Â2] metallic grid. Journal of Molecular Structure, 2021, 1225, 129269.	1.8	4
1478	London Dispersion Interactions Rather than Steric Hindrance Determine the Enantioselectivity of the Corey–Bakshi–Shibata Reduction. Angewandte Chemie, 2021, 133, 4873-4882.	1.6	10
1479	Rotational spectrum and internal dynamics of the hydrogen-bonded pyrrole-pyridine aromatic pair. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 249, 119320.	2.0	1
1480	In Silico Study of Coumarins and Quinolines Derivatives as Potent Inhibitors of SARS-CoV-2 Main Protease. Frontiers in Chemistry, 2020, 8, 595097.	1.8	28
1481	Sensing Mechanism of <scp>Excited‣tate</scp> Intermolecular Hydrogen Bond for Phthalimide: Indispensable Role of Dimethyl Sulfoxide. Chinese Journal of Chemistry, 2021, 39, 1113-1120.	2.6	3
1482	Conformational analysis and electronic interactions of some 2- [2′-(4′-sustituted-phenylsulfanyl)-acetyl]-5-substituted furans and 2- [2′-(phenylselanyl)-acetyl]-5-methylfuran. Journal of Molecular Structure, 2021, 1225, 129088.	1.8	2
1483	Intramolecular London Dispersion Interactions Do Not Cancel in Solution. Journal of the American Chemical Society, 2021, 143, 41-45.	6.6	53
1484	Interplay of weak noncovalent interactions in alkoxybenzylidene derivatives of benzohydrazide and acetohydrazide: a combined experimental and theoretical investigation and lipoxygenase inhibition (LOX) studies. CrystEngComm, 2021, 23, 955-971.	1.3	9
1485	Synthesis and characterization of N-heterocyclic carbene–Mâ‹⁻OEt < sub > 2 < /sub > complexes (M = Cu, Ag,) Tj E <sup>-</sup> Chemical Physics, 2021, 23, 1577-1583.	Qq1 1 0. 1.3	784314 rg₿⊺ 3
1486	Energetically significant cooperative π-stacked ternary assemblies in Ni(II) phenanthroline compounds involving discrete water clusters: Anticancer activities and theoretical studies. Journal of Molecular Structure, 2021, 1229, 129486.	1.8	17
1487	Derivation of an accurate geometry of 2-fluoroaniline from rotational spectroscopy and computational chemistry. Journal of Molecular Structure, 2021, 1225, 129100.	1.8	2

#	Article	IF	CITATIONS
1488	In silico study of the adsorption of acetamiprid on functionalized carbon nanocones. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 128, 114516.	1.3	11
1489	Energetically significant anti-parallel π-stacking and unconventional anion-π interactions in phenanthroline based Ni(II) and Cu(II) coordination compounds: Antiproliferative evaluation and theoretical studies. Inorganica Chimica Acta, 2021, 516, 120082.	1.2	16
1490	IRMOF â€8: Theoretical evaluation of aluminum doping on hydrogen, methane, and hydrogen sulfide adsorption. International Journal of Quantum Chemistry, 2021, 121, e26510.	1.0	6
1491	Theoretical designing and understanding of the performances of BH bridged organocatalysts by Ï€â€conjugated molecules in CO 2 hydroboration. International Journal of Quantum Chemistry, 2021, 121, e26512.	1.0	3
1492	Stability of spherical molecular complexes: a theoretical study of self-assembled M12L24 nanoballs. Structural Chemistry, 2021, 32, 775-785.	1.0	2
1493	Reappraising Schmidpeter's bis(iminophosphoranyl)phosphides: coordination to transition metals and bonding analysis. Chemical Science, 2021, 12, 253-269.	3.7	7
1494	Reduction of peroxynitrite by some manganoporphyrins of AEOL series: DFT approach with dispersion correction and NBO analysis. Journal of Inorganic Biochemistry, 2021, 214, 111299.	1.5	2
1495	Existence of stronger C H···π(chelate ring) interaction compared to C H···π(arene) interactions in the supramolecular assembly of dinuclear iron(III) Schiff base complexes: A theoretical insight. Inorganica Chimica Acta, 2021, 516, 120081.	1.2	9
1496	<scp>NCIPLOT</scp> and the analysis of noncovalent interactions using the reduced density gradient. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1497.	6.2	56
1497	Theoretical study of new LmDHODH and LmTXNPx complexes: structure-based relationships. Structural Chemistry, 2021, 32, 167-177.	1.0	12
1498	Growth behavior and properties of (HF)1–16 clusters. Structural Chemistry, 2021, 32, 395-403.	1.0	6
1499	Efficient hydro-finishing of polyalfaolefin based lubricants under mild reaction condition using Pd on ligands decorated halloysite. Journal of Colloid and Interface Science, 2021, 581, 939-953.	5.0	56
1500	Exploring Epigenetic Marks by Analysis of Noncovalent Interactions. ChemBioChem, 2021, 22, 408-415.	1.3	2
1501	Coinage-metal pillarplexes hosts. Insights into host–guest interaction nature and luminescence quenching effects. Physical Chemistry Chemical Physics, 2021, 23, 15917-15924.	1.3	7
1502	Exploiting the role of stereoelectronic effects to design the antagonists of the human complement C3a receptor. New Journal of Chemistry, 2021, 45, 9443-9455.	1.4	2
1503	Designing high performance conjugated materials for photovoltaic cells with the aid of intramolecular noncovalent interactions. Chemical Communications, 2021, 57, 302-314.	2.2	65
1504	O–H stretching frequency red shifts do not correlate with the dissociation energies in the dimethylether and dimethylsulfide complexes of phenol derivatives. Physical Chemistry Chemical Physics, 2021, 23, 5718-5739.	1.3	4
1505	Anion-dependent structural variations and charge transport property analysis of 4′-(3-pyridyl)-4,2′:6′,4′′-terpyridinium salts. CrystEngComm, 2021, 23, 3569-3581.	1.3	5

#	Article	IF	CITATIONS
1506	Insight into non-covalent interactions in two triamine-based mononuclear iron( <scp>iii</scp> ) Schiff base complexes with special emphasis on the formation of Brâ<ï€ halogen bonding. CrystEngComm, 2021, 23, 1578-1587.	1.3	8
1507	Ultrashort Hδ+â⊄Hδâ^' intermolecular distance in a supramolecular system in the solid state. Chemical Communications, 2021, 57, 7112-7115.	2.2	4
1508	Supramolecular assemblies involving biologically relevant antiparallel π-stacking and unconventional solvent driven structural topology in maleato and fumarato bridged Zn( <scp>ii</scp> ) coordination polymers: antiproliferative evaluation and theoretical studies. New Journal of Chemistry, 2021, 45, 13040-13055.	1.4	9
1509	Unveiling the role of pyrylium frameworks on π-stacking interactions: a combined <i>ab initio</i> and experimental study. Physical Chemistry Chemical Physics, 2022, 24, 1965-1973.	1.3	1
1510	Effect of noncovalent interactions in ion pairs on hypervalent iodines: inversion of regioselectivity in sulfonyloxylactonization. Organic Chemistry Frontiers, 2021, 8, 3695-3704.	2.3	3
1511	Exploring the non-covalent interactions behind the formation of amine–water complexes: the case of <i>N</i> -allylmethylamine monohydrate. Physical Chemistry Chemical Physics, 2021, 23, 7368-7375.	1.3	5
1512	An experimental and theoretical exploration of supramolecular interactions and photoresponse properties of two Ni( <scp>ii</scp> ) complexes. New Journal of Chemistry, 2021, 45, 12108-12119.	1.4	8
1513	Trinuclear molybdenum clusters with sulfide bridges as potential anionic receptors <i>via</i> chalcogen bonding. CrystEngComm, 2021, 23, 4607-4614.	1.3	6
1514	Synthesis and characterization of a mononuclear zinc( <scp>ii</scp> ) Schiff base complex: on the importance of C–Hâ<ï€ interactions. RSC Advances, 2021, 11, 30148-30155.	1.7	13
1515	Theoretical study of spodium bonding in the active site of three Zn-proteins and several model systems. Physical Chemistry Chemical Physics, 2021, 23, 16888-16896.	1.3	12
1516	H-Bonds, π-Stacking and (Water)O-H/π Interactions in (µ4-EDTA)Bis(Imidazole) Dicopper(II) Dihydrate. Crystals, 2021, 11, 48.	1.0	4
1517	Cyclopeptides from the Mushroom Pathogen Fungus <i>Cladobotryum varium</i> . Journal of Natural Products, 2021, 84, 327-338.	1.5	9
1518	Classics Meet Classics: Theoretical and Experimental Studies of Halogen Bonding in Adducts of Platinum(II) 1,5-Cyclooctadiene Halide Complexes with Diiodine, Iodoform, and 1,4-Diiodotetrafluorobenzene. Crystal Growth and Design, 2021, 21, 974-987.	1.4	15
1519	Insights into the kinetics and molecular mechanism of the Newman–Kwart rearrangement. New Journal of Chemistry, 2021, 45, 16978-16988.	1.4	2
1520	Synthesis, X-ray characterization and theoretical study of all-cis 1,4:2,3:5,8:6,7-tetraepoxynaphthalenes: on the importance of through-space α-effect. CrystEngComm, 0, , .	1.3	2
1521	Replacing thymine with a strongly pairing fifth Base: A combined quantum mechanics and molecular dynamics study. Computational and Structural Biotechnology Journal, 2021, 19, 1312-1324.	1.9	12
1522	Photoinduced electron transfer in nano-Saturn complexes of fullerene. Physical Chemistry Chemical Physics, 2021, 23, 2126-2133.	1.3	8
1523	Crystal engineering with pyrazolyl-thiazole derivatives: structure-directing role of Ï€-stacking and Ïf-hole interactions. CrystEngComm, 2021, 23, 3276-3287.	1.3	21

#	Article	IF	CITATIONS
1524	Mechanism and regio- and stereoselectivity in an NHC-catalyzed Mannich/lactamization domino reaction. Physical Chemistry Chemical Physics, 2021, 23, 6204-6212.	1.3	7
1525	Comprehensive defect suppression in perovskite nanocrystals for high-efficiency light-emitting diodes. Nature Photonics, 2021, 15, 148-155.	15.6	590
1526	Novel cationic 1,2,4-selenadiazoles: synthesis <i>via</i> addition of 2-pyridylselenyl halides to unactivated nitriles, structures and four-center Seâ <n 2021,="" 50,<br="" contacts.="" dalton="" transactions,="">10689-10691.</n>	1.6	22
1527	Towards the understanding of halogenation in peptide hydrogels: a quantum chemical approach. Materials Advances, 2021, 2, 4792-4803.	2.6	3
1528	A theoretical insight on the anionâ<ānion interactions observed in the solid state structure of a hetero-trinuclear complex. CrystEngComm, 2021, 23, 1429-1438.	1.3	11
1529	DFT study of H <sub>2</sub> adsorption at a Cu-SSZ-13 zeolite: a cluster approach. Physical Chemistry Chemical Physics, 2021, 23, 9980-9990.	1.3	16
1530	Experimental and Theoretical Studies of Dimers Stabilized by Two Chalcogen Bonds in the Presence of a N··À·N Pnicogen Bond. Journal of Physical Chemistry A, 2021, 125, 657-668.	1.1	14
1531	Intramolecular aurophilic interactions in dinuclear gold( <scp>i</scp> ) complexes with twisted bridging 2,2′-bipyridine ligands. Dalton Transactions, 2021, 50, 12448-12456.	1.6	17
1532	Interactions of aromatic rings in the crystal structures of hybrid polyoxometalates and Ru clusters. CrystEngComm, 2021, 23, 6409-6417.	1.3	9
1533	Theoretical evaluation of the performance of IRMOFs and M-MOF-74 in the formation of 5-fluorouracil@MOF. RSC Advances, 2021, 11, 31090-31097.	1.7	11
1534	Molecular Dynamics Simulations of Self-Healing Topological Copolymers with a Comblike Structure. Macromolecules, 2021, 54, 1095-1105.	2.2	24
1535	On the importance of RH <sub>3</sub> Câ< N tetrel bonding interactions in the solid state of a dinuclear zinc complex with a tetradentate Schiff base ligand. CrystEngComm, 2021, 23, 3391-3397.	1.3	8
1536	5-Methoxy-1-methyl-2-{[4-(2-hydroxyphenyl)piperazin-1-yl]methyl}-1Hindole (KAD22) with Antioxidant Activity. Letters in Organic Chemistry, 2021, 18, .	0.2	0
1537	A case study of Pdâ‹ <sup>-</sup> Pd intramolecular interaction in a benzothiazole based palladacycle; catalytic activity toward amide synthesis <i>via</i> an isocyanide insertion pathway. New Journal of Chemistry, 2021, 45, 3290-3297.	1.4	5
1538	Differentiating intramolecular spodium bonds from coordination bonds in two polynuclear zinc( <scp>ii</scp> ) Schiff base complexes. CrystEngComm, 2021, 23, 2703-2710.	1.3	39
1539	Towards developing a criterion to characterize non-covalent bonds: a quantum mechanical study. Physical Chemistry Chemical Physics, 2021, 23, 8478-8488.	1.3	29
1540	Systematic Search for Transition States in Complex Molecules: Computational Analyses of Regio- and Stereoselective Interflavan Bond Formation in Flavan-3-ols. Heterocycles, 2021, 102, 1061.	0.4	2
1541	A bifunctional iminophosphorane squaramide catalyzed enantioselective synthesis of hydroquinazolines <i>&gt;via</i> intramolecular aza-Michael reaction to î±,î²-unsaturated esters. Chemical Science, 2021, 12, 6064-6072.	3.7	21

	CITATION REI	PORT	
#	Article	IF	CITATIONS
1542	"Anti-electrostatic―halogen bonding in solution. Chemical Science, 2021, 12, 8246-8251.	3.7	20
1543	Biological halogen bonds in protein–ligand complexes: a combined QTAIM and NCIPlot study in four representative cases. Organic and Biomolecular Chemistry, 2021, 19, 6858-6864.	1.5	10
1544	1-Alkyl-3-methylimidazolium cation binding preferences in hexafluorophosphate ionic liquid clusters determined using competitive TCID measurements and theoretical calculations. Physical Chemistry Chemical Physics, 2021, 23, 18145-18162.	1.3	4
1545	Direct evidence for distinct colour origins in ROY polymorphs. Chemical Science, 2021, 12, 12711-12718.	3.7	13
1546	A Step toward the Quantification of Noncovalent Interactions in Large Biological Systems: The Independent Gradient Model-Extremely Localized Molecular Orbital Approach. Journal of Chemical Information and Modeling, 2021, 61, 795-809.	2.5	13
1547	Theoretical model for N-heterocyclic carbene-catalyzed decarboxylation reactions. Organic Chemistry Frontiers, 2021, 8, 3268-3273.	2.3	19
1548	Spodium bonding in five coordinated Zn( <scp>ii</scp> ): a new player in crystal engineering?. CrystEngComm, 2021, 23, 3084-3093.	1.3	33
1549	Biologically relevant and energetically significant cooperative ternary (Ĩ€â€"Ĩ€)2/(Ĩ€â€"Ĩ€)1/(Ĩ€â€"Ĩ€)2 assemblies and fascinating discrete (H2O)21 clusters in isostructural 2,5-pyridine dicarboxylato Co(ii) and Zn(ii) phenanthroline compounds: antiproliferative evaluation and theoretical studies. New Journal of Chemistry. 2021. 45. 3699-3715.	1.4	13
1550	Unusual π–π interactions directed by the [{(C <sub>6</sub> H <sub>6</sub> )Ru} <sub>2</sub> W <sub>8</sub> O <sub>30</sub> (OH) <sub>2</sub> ] <sup hybrid anion. CrystEngComm, 2021, 23, 4125-4135.</sup 	> <b>6.â^'</b> <td>ряз</td>	ряз
1551	Inclusion of capecitabine into cucurbiturils: DFT study for supramolecular encapsulation of anticancer drug. Monatshefte Für Chemie, 2021, 152, 209-216.	0.9	1
1552	Interplay between non-covalent interactions in 1D supramolecular polymers based on 1,4-bis(iodoethynyl)benzene. Physical Chemistry Chemical Physics, 2021, 23, 3531-3542.	1.3	3
1553	Possible effects of fluxionality of a cavitand on its catalytic activity through confinement. Physical Chemistry Chemical Physics, 2021, 23, 15817-15834.	1.3	5
1554	Tricyclic systems: Central Carbon Ring With Fused Six-Membered Rings. , 2022, , 1020-1043.		2
1555	Mechanistic study on the NHC-catalyzed [3+4] annulation of enals and thiazolones. New Journal of Chemistry, 2021, 45, 12129-12137.	1.4	7
1556	Commentary toward the 20th Anniversary of the Society ofComputer Chemistry, Japan. Journal of Computer Chemistry Japan, 2021, 20, A26-A40.	0.0	0
1557	Insights into the Mechanism of Low-Valent Cobalt-Catalyzed C–H Activation. ACS Catalysis, 2021, 11, 1505-1515.	5.5	32
1558	Alkaline earth atom doping-induced changes in the electronic and magnetic properties of graphene: a density functional theory study. RSC Advances, 2021, 11, 6268-6283.	1.7	10
1559	Insights into the chiral sulfide/selenide-catalyzed electrophilic carbothiolation of alkynes: mechanism and origin of axial chirality. Organic Chemistry Frontiers, 2021, 8, 1983-1990.	2.3	20

#	Article	IF	CITATIONS
1560	A theoretical insight into the formation of chalcogen bonding (ChB) interactions involving coordinated DMSO molecules as Ï <i>f</i> -hole donors and benzoate groups as Ï <i>f</i> -hole acceptors in a dinuclear copper( <scp>ii</scp> ) complex. CrystEngComm, 2021, 23, 5087-5096.	1.3	12
1561	Nucleophilic iodonium interactions (NIIs) in 2-coordinate iodine( <scp>i</scp> ) and silver( <scp>i</scp> ) complexes. Chemical Communications, 2021, 57, 5094-5097.	2.2	13
1562	Theoretical introduction and design of Si/N catalysts as efficient reducing agents in CO2 hydroboration by planar Si/N π-conjugated molecules. Structural Chemistry, 2021, 32, 1327-1340.	1.0	2
1563	X-ray characterization, Hirshfeld surface analysis, DFT calculations, <i>in vitro</i> and <i>in silico</i> lipoxygenase inhibition (LOX) studies of dichlorophenyl substituted 3-hydroxy-chromenones. New Journal of Chemistry, 2021, 45, 19928-19940.	1.4	22
1564	A quantum crystallographic approach to short hydrogen bonds. CrystEngComm, 2021, 23, 6180-6190.	1.3	10
1565	Spontaneous bond dissociation cascades induced by Be <sub>n</sub> clusters ( <i>n</i> = 2,4). Physical Chemistry Chemical Physics, 2021, 23, 6448-6454.	1.3	3
1566	1,3,4-Oxadiazole-functionalized <i>α</i> -amino-phosphonates as ligands for the ruthenium-catalyzed reduction of ketones. New Journal of Chemistry, 2021, 45, 11327-11335.	1.4	12
1567	Insight into the formation of H-bonds propagating the monomeric zinc complexes of a tridentate reduced Schiff base to form an infinite chain. CrystEngComm, 2021, 23, 1918-1928.	1.3	6
1568	An Androsteroneâ€H <sub>2</sub> @C <sub>60</sub> hybrid: Synthesis, Properties and Molecular Docking Simulations with SARSâ€Covâ€2. ChemPlusChem, 2021, 86, 972-981.	1.3	9
1569	Bifurcated Halogen Bonding Involving Two Rhodium(I) Centers as an Integrated σ-Hole Acceptor. Jacs Au, 2021, 1, 354-361.	3.6	39
1570	Intermolecular Interactions between Thiocyanato Ligands in Metal Complexes. Crystal Growth and Design, 2021, 21, 1636-1644.	1.4	4
1571	Insights into the Chiral Phosphoric Acid-Catalyzed Dynamic Kinetic Asymmetric Hydroamination of Racemic Allenes: An Allyl Carbocation/Phosphate Pair Mechanism. Journal of Organic Chemistry, 2021, 86, 4121-4130.	1.7	8
1572	A Theoretical Study on the Degenerate Cope Rearrangement of Hypostrophene Using the RRKM Theory and Topological Approaches. ChemistrySelect, 2021, 6, 1607-1615.	0.7	1
1573	Fluorination Effects in XPhos Gold(I) Fluorothiolates. Inorganics, 2021, 9, 14.	1.2	1
1574	Synthesis, in silico, and in vitro studies of novel dopamine D 2 and D 3 receptor ligands. Archiv Der Pharmazie, 2021, 354, 2000486.	2.1	7
1575	Size-Driven Inversion of Selectivity in Esterification Reactions: Secondary Beat Primary Alcohols. Journal of Organic Chemistry, 2021, 86, 3456-3489.	1.7	4
1577	Comprehensive Bonding Analysis of Tetravalent f-Element Complexes of the Type [M(salen) <sub>2</sub> ]. Inorganic Chemistry, 2021, 60, 2514-2525.	1.9	23
1578	Synthesis, docking studies, and pharmacological evaluation of 2â€hydroxypropylâ€4â€arylpiperazine derivatives as serotoninergic ligands. Archiv Der Pharmazie, 2021, 354, 2000414.	2.1	7

#	Article	IF	CITATIONS
1579	Extending Libraries of Extremely Localized Molecular Orbitals to Metal Organic Frameworks: A Preliminary Investigation. Crystals, 2021, 11, 207.	1.0	4
1580	A theoretical study to the loliolide molecule and its isomers: a study by circular dichroism, QTAIM, and NMR theoretical methods. Journal of Molecular Modeling, 2021, 27, 116.	0.8	2
1581	Revealing new non-covalent interactions in polymorphs and hydrates of Acyclovir: Hirshfeld surface analysis, NCI plots and energetic calculations. Computational and Theoretical Chemistry, 2021, 1197, 113133.	1.1	7
1582	Microhydration of ionized building blocks of DNA/RNA: infrared spectra of pyrimidine\$\$^{+}\$\$-\$\$(hbox {H}_{2}hbox {O})_{ext {1-3}}\$\$ clusters. European Physical Journal D, 2021, 75, 1.	0.6	1
1583	Multiple Functional Organocatalyst-Promoted Inert C–C Activation: Mechanism and Origin of Selectivities. ACS Catalysis, 2021, 11, 3443-3454.	5.5	38
1584	Nonuniform Proton Transfer and Strong Hydrogen Bonding within Cation, Anion, and Neutral Clusters of Ammonia and Hydrogen Fluoride. Journal of Physical Chemistry A, 2021, 125, 2546-2557.	1.1	2
1585	Combined Theoretical and Experimental Investigation of Lewis Acid-Carbonyl Interactions for Metathesis. ACS Catalysis, 2021, 11, 4381-4394.	5.5	6
1586	Weak Interactions in Cocrystals of Isoniazid with Glycolic and Mandelic Acids. Crystals, 2021, 11, 328.	1.0	8
1587	Synergistically improving myricetin ESIPT and antioxidant activity via dexterously trimming atomic electronegativity. Journal of Molecular Liquids, 2021, 325, 115272.	2.3	26
1588	Exploring the Structure–Performance Relationship of Sulfonated Polysulfone Proton Exchange Membrane by a Combined Computational and Experimental Approach. Polymers, 2021, 13, 959.	2.0	18
1589	Screening Nanographeneâ€Mediated Inter(Porphyrin) Communication to Optimize Inter(Porphyrin–Fullerene) Forces. Advanced Energy Materials, 2021, 11, 2100158.	10.2	9
1590	How the water-soluble hemicarcerand incarcerates guests at room temperature decoded with modular simulations. Communications Chemistry, 2021, 4, .	2.0	1
1591	Deciphering the H-Bonding Preference on Nucleoside Molecular Recognition through Model Copper(II) Compounds. Pharmaceuticals, 2021, 14, 244.	1.7	4
1592	Highly Sterically Encumbered Gold Acyclic Diaminocarbene Complexes: Overriding Electronic Control in Regiodivergent Gold Catalysis. Organometallics, 2021, 40, 1416-1433.	1.1	10
1593	Supramolecular organic frameworks derived from bromoaryl-substituted dichlorodiazabutadienes via Cl···Br halogen bonding. Mendeleev Communications, 2021, 31, 191-193.	0.6	19
1594	Noncovalent Interactions between Stacked Arenes in 1,8â€Bisâ€(1â€naphthyl)â€naphthalenes. European Journal of Organic Chemistry, 2021, 2021, 2594-2603.	1.2	3
1595	NanoMIPs Design for Fucose and Mannose Recognition: A Molecular Dynamics Approach. Journal of Chemical Information and Modeling, 2021, 61, 2048-2061.	2.5	6
1596	IDENTIFICATION OF SUPRAMOLECULAR DIMERS IN THE CRYSTAL STRUCTURE OF (Z)-1-(((5-FLUOROPYRIDIN-2-YL)AMINO)METHYLENE)NAPHTHALEN-2(1H)-ONE via C(sp2)–Hâ <f hydrogen<br="">BONDING: A COMBINED EXPERIMENTAL AND THEORETICAL STUDY. Journal of Structural Chemistry, 2021, 62, 460-466.</f>	0.3	5

#	Article	IF	CITATIONS
1597	Quantum Mechanical Calculations for Biomass Valorization over Metalâ€Organic Frameworks (MOFs). Chemistry - an Asian Journal, 2021, 16, 1049-1056.	1.7	7
1598	Rotational spectrum and quantum chemical calculations of methyl cyanoacetate: A compound of potential astrochemical interest. Journal of Molecular Spectroscopy, 2021, 377, 111444.	0.4	5
1600	Dynamic chiral self-recognition in aromatic dimers of styrene oxide revealed by rotational spectroscopy. Communications Chemistry, 2021, 4, .	2.0	8
1601	Ni/Cu-catalyzed silylation of allylic alcohol: Theoretical studies on the mechanisms, regioselectivity, and role of ligand. Molecular Catalysis, 2021, 504, 111456.	1.0	1
1602	Judicious design functionalized <scp>3Dâ€COF</scp> to enhance <scp>CO<sub>2</sub></scp> adsorption and separation. Journal of Computational Chemistry, 2021, 42, 888-896.	1.5	14
1603	Attractive fluorine···fluorine interactions between perfluorinated alkyl chains: a case of perfluorinated Cu(II) diiminate Cu[C <sub>2</sub> F <sub>5</sub> –C(NH)–CF=C(NH)–CF <sub>3</sub> ] <sub>2</sub> . Zeitschrift Fur Kristallographie - Crystalline Materials. 2021. 236. 117-122.	0.4	11
1604	Theoretical investigations on forward–backward ESIPT processes of three fluorophores deriving from 2-(2′-hydroxyphenyl)thiazole. Photochemical and Photobiological Sciences, 2021, 20, 533-546.	1.6	4
1605	Computational Study on the Structure, Stability, and Electronic Feature Analyses of Trapped Halocarbons inside a Novel Bispyrazole Organic Molecular Cage. ACS Omega, 2021, 6, 11711-11728.	1.6	7
1606	Polymorphs of 2-[2-[(2,6-dichlorophenyl)amino]phenyl]acetic acid (Diclofenac): Differences from crystallography, Hirshfeld surface, QTAIM and NCIPlots. Chemical Physics, 2021, 544, 111119.	0.9	4
1607	Characterization of Large-Amplitude Motions and Hydrogen Bonding Interactions in the Thiophene–Water Complex by Rotational Spectroscopy. Journal of Physical Chemistry A, 2021, 125, 3425-3431.	1.1	8
1608	Atom-Efficient Halogen–Halogen Interactions Assist One-, Two-, and Three-Dimensional Molecular Zippers. Journal of Physical Chemistry C, 2021, 125, 10716-10722.	1.5	6
1609	Theoretical study of the interplay between double chalcogen-bonding interactions and halogen bonds in ditopic molecular module systems. Computational and Theoretical Chemistry, 2021, 1198, 113182.	1.1	3
1610	Development of a Nanostructured Lipid Carrier (NLC) by a Low-Energy Method, Comparison of Release Kinetics and Molecular Dynamics Simulation. Pharmaceutics, 2021, 13, 531.	2.0	27
1611	Focal Point Evaluation of Energies for Tautomers and Isomers for 3-hydroxy-2-butenamide: Evaluation of Competing Internal Hydrogen Bonds of Types -OH…O=, -OH…N, -NH…O=, and CH…X (X=O and N). Molecules, 2021, 26, 2623.	1.7	3
1612	Theoretical investigation of X12O12 (XÂ=ÂBe, Mg, and Ca) in sensing CH2N2: A DFT study. Computational and Theoretical Chemistry, 2021, 1198, 113168.	1.1	35
1613	A computational investigation of the selectivity and mechanism of the Lewis acid catalyzed oxaâ€Diels–Alder cycloaddition of substituted diene with benzaldehyde. Journal of Computational Chemistry, 2021, 42, 1296-1311.	1.5	10
1614	Azine Steric Hindrances Switch Halogen Bonding to <i>N</i> â€Arylation upon Interplay with σâ€Hole Donating Haloarenenitriles. Chemistry - an Asian Journal, 2021, 16, 1445-1455.	1.7	9
1616	Crystal structure determination and computational studies of 1,4-dihydropyridine derivatives as selective T-type calcium channel blockers. Journal of Molecular Structure, 2021, 1230, 129898.	1.8	8

	CITATION REF	ORT	
#	Article	IF	CITATIONS
1617	(6-Diphenylphosphinoacenaphth-5-yl)indium and -nickel Compounds: Synthesis, Structure, Transmetalation, and Cross-Coupling Reactions. Organometallics, 2021, 40, 1284-1295.	1.1	5
1618	Effective adsorption of A-series chemical warfare agents on graphdiyne nanoflake: a DFT study. Journal of Molecular Modeling, 2021, 27, 117.	0.8	26
1619	Conformational preferences of diallylamine: A rotational spectroscopic and theoretical study. Journal of Chemical Physics, 2021, 154, 164303.	1.2	3
1620	Stereochemical Control of Tricoordinate Copper(I) Complexes Based on N-(9-Alkyl-9-fluorenyl)-Substituted Heterocyclic Carbenes. Synthesis, 2021, 53, 1785-1794.	1.2	1
1622	Nanotechnology-based approaches for targeting and delivery of drugs via Hexakis (m-PE) macrocycles. Scientific Reports, 2021, 11, 8256.	1.6	11
1623	Enantioselectivity in the Noyori–Ikariya Asymmetric Transfer Hydrogenation of Ketones. Organometallics, 2021, 40, 1402-1410.	1.1	24
1624	Pillar[5]arene-Derived <i>endo</i> -Functionalized Molecular Tube for Mimicking Protein–Ligand Interactions. Journal of Organic Chemistry, 2021, 86, 6467-6477.	1.7	7
1625	Study of Beryllium, Magnesium, and Spodium Bonds to Carbenes and Carbodiphosphoranes. Molecules, 2021, 26, 2275.	1.7	18
1626	Interaction–Deletion: A Composite Energy Method for the Optimization of Molecular Systems Selectively Removing Specific Nonbonded Interactions. Journal of Physical Chemistry A, 2021, 125, 4668-4682.	1.1	0
1627	The Adsorption of 1-Chloro-1,2,2,2-Tetrafluoroethane Onto the Pristine, Al-, and Ga-Doped Boron Nitride Nanosheet. Iranian Journal of Science and Technology, Transaction A: Science, 2021, 45, 1287-1300.	0.7	29
1628	High-Strength, Strongly Bonded Nanocomposite Hydrogels for Cartilage Repair. ACS Applied Materials & Interfaces, 2021, 13, 24505-24523.	4.0	50
1629	Computational considerations on the mechanism and stereoselectivity in cyclopropanation reactions via iron-carbenes. Tetrahedron Letters, 2021, 72, 153023.	0.7	1
1630	A DFT study on the mechanism and selectivity of [3 + 2] cycloaddition reactions leading to pyrole[2,1-a] phthalazine compounds. Theoretical Chemistry Accounts, 2021, 140, .	0.5	1
1631	Stepwise Microhydration of Isoxazole: Infrared Spectroscopy of Isoxazole-(Water) <sub><i>n</i>â‰ਊ</sub> Clusters in Helium Nanodroplets. Journal of Physical Chemistry A, 2021, 125, 4766-4774.	1.1	3
1632	Carbo â€mer of Barrelene: A Rigid 3Dâ€Carbonâ€Expanded Molecular Barrel. Chemistry - A European Journal, 2021, 27, 9286-9291.	1.7	2
1633	London Dispersion Helps Refine Steric A-Values: The Halogens. Journal of Organic Chemistry, 2021, 86, 7701-7713.	1.7	14
1634	Robust, Enantioselective Construction of Challenging, Biologically Relevant Tertiary Ether Stereocenters. ACS Catalysis, 2021, 11, 6325-6333.	5.5	17
1635	Synthesis of Chiral α-Amino Tertiary Boronates via the Catalytic Enantioselective Nucleophilic Borylation of Dialkyl Ketimines. ACS Catalysis, 2021, 11, 6733-6740.	5.5	12

#	Article	IF	CITATIONS
1636	Exploring Li4N and Li4O superalkalis as efficient dopants for the Al12N12 nanocage to design high performance nonlinear optical materials with high thermodynamic stability. Polyhedron, 2021, 200, 115145.	1.0	12
1637	How Many Electrons Does a Molecular Electride Hold?. Journal of Physical Chemistry A, 2021, 125, 4819-4835.	1.1	7
1638	Iodine atalyzed Dielsâ€Alder Reactions. ChemCatChem, 2021, 13, 2922-2930.	1.8	12
1639	Insights into the selective sensing mechanism of a luminescent Cd(II)-based MOF chemosensor toward NACs: roles of the host–guest interactions and PET processes. Journal of Materials Science, 2021, 56, 13684-13704.	1.7	14
1641	How Do Defects in Carbon Nanostructures Regulate the Photoinduced Electron Transfer Processes? The Case of Phenine Nanotubes. ChemPhysChem, 2021, 22, 1178-1186.	1.0	7
1642	Copper and neurodegenerative disorders: potential drugs for possible successful treatment. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	5
1643	The Crystal Structure and Intermolecular Interactions in Fenamic Acids–Acridine Complexes. Molecules, 2021, 26, 2956.	1.7	4
1644	Exploring weak intermolecular interactions in two bis-1,3,4-oxadiazoles derivatives: A combined X-ray diffraction, Hirshfeld surface analysis and theoretical studies. Journal of Molecular Structure, 2021, 1232, 130030.	1.8	7
1645	Pd on nitrogen rich polymer–halloysite nanocomposite as an environmentally benign and sustainable catalyst for hydrogenation of polyalfaolefin based lubricants. Journal of Industrial and Engineering Chemistry, 2021, 97, 441-451.	2.9	47
1646	Spodium bonding and other non-covalent interactions assisted supramolecular aggregation in a new mercury(II) complex of a nicotinohydrazide derivative. Inorganica Chimica Acta, 2021, 519, 120279.	1.2	25
1647	From the Design to the <i>In Vivo</i> Evaluation of Benzohomoadamantane-Derived Soluble Epoxide Hydrolase Inhibitors for the Treatment of Acute Pancreatitis. Journal of Medicinal Chemistry, 2021, 64, 5429-5446.	2.9	12
1648	Mechanistic Study of Ni and Cu Dual Catalyst for Asymmetric C–C Bond Formation; Asymmetric Coupling of 1,3-Dienes with C-nucleophiles to Construct Vicinal Stereocenters. ACS Catalysis, 2021, 11, 6643-6655.	5.5	52
1649	Bulk and Surface Conformations in Solid-State Lovastatin: Spectroscopic and Molecular Dynamics Studies. Crystals, 2021, 11, 509.	1.0	1
1650	Fluxional bis(phenoxy-imine) Zr and Ti catalysts for polymerization. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	2
1651	Complex formation of titanocene dichloride anticancer and Al12N12 nano-cluster: A quantum chemical investigation of solvent, temperature and pressure effects. Main Group Chemistry, 2021, 20, 19-32.	0.4	4
1652	Asymmetric Nucleophilic Allylation of α-Chloro Glycinate via Squaramide Anion-Abstraction Catalysis: S <sub>N</sub> 1 or S <sub>N</sub> 2 Mechanism, or Both?. Journal of Organic Chemistry, 2021, 86, 8414-8424.	1.7	5
1653	An NHCâ€Stabilised Phosphinidene for Catalytic Formylation: A DFTâ€Guided Approach. Chemistry - A European Journal, 2021, 27, 11656-11662.	1.7	6
1654	Evaluation of Electron Density Shifts in Noncovalent Interactions. Journal of Physical Chemistry A, 2021, 125, 4741-4749.	1.1	15

#	Article		CITATIONS
1655	An insight to the spin density distribution and non-covalent interactions in a carboxylate bridged class-I mixed valence cobalt(II),cobalt(III) complex of quadruplet nature. Inorganica Chimica Acta, 2021, 521, 120298.	1.2	8
1656	Coordination from Heteroscorpionate Ligand Towards Pd(II) via Pdâ‹â‹Ĥr̂á^'C(sp3) Interaction: Structural and Catalytic Studies. European Journal of Inorganic Chemistry, 2021, 2021, 2661-2668.	1.0	3
1657	Structural Diversity and Argentophilic Interactions in Small Phosphine Silver(I) Thiolate Clusters. European Journal of Inorganic Chemistry, 2021, 2021, 2702-2711.	1.0	9
1658	Different Reactivities of (5-Ph <sub>2</sub> P-Ace-6-) <sub>2</sub> MeSiH toward the Rhodium(I) Chlorides [(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> RhCl] <sub>2</sub> and [(CO) <sub>2</sub> RhCl] <sub>2</sub> RhCl] <sub>2</sub> RhCl] <sub>2</sub> After action. Organometallics, 2021, 40, 2027-2038.	1.1	6
1659	N-(3-{4-[3-(trifluoromethyl)phenyl]piperazin-1-yl}propyl)-1H-indazole-3-carboxamide (D2AAK3) as a potential antipsychotic: In vitro, in silico and in vivo evaluation of a multi-target ligand. Neurochemistry International, 2021, 146, 105016.	1.9	10
1660	Photochemical Properties and Stability of BODIPY Dyes. International Journal of Molecular Sciences, 2021, 22, 6735.	1.8	17
1661	Theoretical study of the [3Â+Â4] annulation reaction of 2-bromoenals with malonates catalyzed by N-heterocyclic carbene. Molecular Catalysis, 2021, 509, 111647.	1.0	2
1662	Mechanistic Study of Domino Processes Involving the Bidentate Lewis Acid Catalyzed Inverse Electronâ€Đemand Dielsâ^'Alder Reaction. European Journal of Organic Chemistry, 2021, 2021, 3866-3873.	1.2	4
1663	Distinct roles of Ag(I) and Cu(II) as cocatalysts in the intramolecular cyclization of N-methyl-N-phenylanthranilic acid: A theoretical investigation. Molecular Catalysis, 2021, 509, 111634.	1.0	0
1664	Perturbating Intramolecular Hydrogen Bonds through Substituent Effects or Non-Covalent Interactions. Molecules, 2021, 26, 3556.	1.7	6
1665	Pathway Bifurcations in the Activation of Allylic Halides by Palladium and Their Influence on the Dynamics of η <sup>1</sup> and η <sup>3</sup> Allyl Intermediates. Journal of Organic Chemistry, 2021, 86, 9637-9650.	1.7	9
1666	Spectroscopic and Computational Studies on a Dansyl Based Luminescent Probe: Detection of Water Contaminant in Hygroscopic Deuterated Solvents. Letters in Organic Chemistry, 2022, 19, 71-82.	0.2	2
1667	A deep insight into polybenzoxazole formation in the heterocycle-containing polybenzoxazine: An enlightening thought for smarter precursor design. Polymer, 2021, 226, 123789.	1.8	5
1668	Monoprotonated Dimethyl Sulfoxide, [HOSMe 2 ] + : Synthesis, Crystal Structure, Spectroscopic and Theoretical Studies of [HOSMe 2 ] 2 [OsCl 6 ] â‹â€‰2H 2 O. ChemistrySelect, 2021, 6, 5211-5217.	0.7	4
1669	Heptadentate, Octadentate, Or Even Nonadentate? Denticity in the Unexpected Formation of an All-Carbon Donor-Atom Ligand in Rh <sup>III</sup> (Cp*)(Anthracenyl-NHC) Complexes. Inorganic Chemistry, 2021, 60, 8734-8741.	1.9	7
1670	When a "Dimroth Rearrangement―ls Not a Dimroth Rearrangement. Journal of Organic Chemistry, 2021, 86, 8286-8294.	1.7	10
1671	A Halomanganates(II) with P,P'-Diprotonated Bis(2-Diphenylphosphinophenyl)ether: Wavelength-Excitation Dependence of the Quantum Yield and Role of the Non-Covalent Interactions. International Journal of Molecular Sciences, 2021, 22, 6873.	1.8	8
1672	Favipiravir: insight into the crystal structure, Hirshfeld surface analysis and computational study. Journal of the Iranian Chemical Society, 2022, 19, 85-94.	1.2	26

#	Article	IF	CITATIONS
1673	Towards mild conditions by predictive catalysis via sterics in the Ru-catalyzed hydrogenation of thioesters. Molecular Catalysis, 2021, 510, 111692.	1.0	14
1674	Synthesis, structural characterisation and theoretical studies of a novel pyridazine derivative: Investigations of anti-inflammatory activity and inhibition of α-glucosidase. Journal of Molecular Structure, 2021, 1234, 130177.	1.8	11
1675	Non ovalent Interactions in the Biphenyl Crystal: Is the Planar Conformer a Transition State?. Chemistry - A European Journal, 2021, 27, 11912-11918.	1.7	14
1676	A new coordination polymer constructed from Pb(NO3)2 and a benzylideneisonicotinohydrazide derivative: Coordination-induced generation of a ï€-hole towards a tetrel-bonding stabilized structure. Journal of Molecular Structure, 2021, 1234, 130139.	1.8	11
1677	Solvent behavior of an ionic liquid set around a cellulose lÎ <sup>2</sup> crystallite model through molecular dynamics simulations. Cellulose, 2021, 28, 6767-6795.	2.4	7
1678	Role of Dispersion Interactions in Endohedral TM@(ZnS)12 Structures. ACS Omega, 2021, 6, 16612-16622.	1.6	0
1679	Unveiling Five Naked Structures of Tartaric Acid. Angewandte Chemie, 2021, 133, 17550-17554.	1.6	0
1680	Potential activity of Linezolid against SARS-CoV-2 using electronic and molecular docking study. Journal of Molecular Modeling, 2021, 27, 222.	0.8	6
1681	Substituent Effects on Electride Characteristics of Mg <sub>2</sub> (η <sup>5</sup> -C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> : A Theoretical Study. Journal of Physical Chemistry A, 2021, 125, 6207-6220.	1.1	10
1682	Can metal halides be electron donors in Ïfâ€hole and Ï€â€hole tetrel bonds? Cooperativity with an alkalineâ€earth bond. International Journal of Quantum Chemistry, 2021, 121, e26771.	1.0	1
1683	Combined DFT calculation, Hirshfeld surface analysis, and Energy framework study of non-covalent interactions in the crystal structure of (Z)-5-ethylidene-2-thiohydantoin determined by powder X-ray diffraction. Journal of Molecular Structure, 2021, 1236, 130361.	1.8	2
1684	Modeling the structure and reactivity landscapes of a pyrazole-ammonium ionic derivative using wavefunction-dependent characteristics and screening for potential anti-inflammatory activity. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11190-11202.	2.0	3
1685	The effect of ring aromaticity on ESIPT behavior and photophysical properties of 2-(2′-hydroxyphenyl)- 4-chloromethylthiazole derivatives: A TD-DFT study. Journal of Molecular Liquids, 2021, 334, 116517.	2.3	15
1686	Theoretical study on the noncovalent interactions involving triplet diphenylcarbene. Journal of Molecular Modeling, 2021, 27, 224.	0.8	0
1688	Azoimidazole gold(III) complexes: Synthesis, structural characterization and self-assembly in the solid state. Inorganica Chimica Acta, 2021, 522, 120373.	1.2	24
1689	Atoms in Highly Symmetric Environments: H in Rhodium and Cobalt Cages, H in an Octahedral Hole in MgO, and Metal Atoms Ca-Zn in C20 Fullerenes. Symmetry, 2021, 13, 1281.	1.1	0
1690	Investigation of Structures, QTAIM, RDG, ADMET, and docking properties of SASC compound using experimental and theoretical approach. Computational and Theoretical Chemistry, 2021, 1201, 113287.	1.1	12
1691	Hydrogen bonding networks and cooperativity effects in the aqueous solvation of trimethylene oxide and sulfide rings by microwave spectroscopy and computational chemistry. Journal of Chemical Physics, 2021, 155, 034305.	1.2	4

#	Article	IF	CITATIONS
1692	Adsorption properties of amino acid-based ionic liquids (AAILs) on edge fluorinated graphene surface – a DFT study. Molecular Simulation, 2021, 47, 1066-1077.	0.9	3
1693	Gram-Scale Synthesis of 1,8-Naphthyridines in Water: The Friedlander Reaction Revisited. ACS Omega, 2021, 6, 19304-19313.	1.6	11
1694	Fate of Cobaltacycles in Cp*Co-Mediated C–H Bond Functionalization Catalysis: Cobaltacycles May Collapse upon Oxidation via Co(IV) Species. Organometallics, 2021, 40, 2624-2642.	1.1	4
1695	Excess properties, spectral analyses and computational chemistry of the binary mixture of polyethylene glycol 200Â+Â1,3-propanediamine. Journal of Molecular Liquids, 2022, 346, 117080.	2.3	11
1696	Exploration of the Activation Mechanism of the Epigenetic Regulator MLL3: A QM/MM Study. Biomolecules, 2021, 11, 1051.	1.8	3
1697	Theoretical insights into the directionality of ESIPT behavior of BTHMB molecule with two proton acceptors in solution. Chemical Physics Letters, 2021, 775, 138670.	1.2	8
1698	A New Insight into Non-covalent Interactions in 1,4-Disubstituted 1H-1,2,3-Triazole: Synthesis, X-ray structure, DFT calculations, in vitro Lipoxygenase Inhibition (LOX) and in silico Studies. Journal of Molecular Structure, 2021, 1236, 130283.	1.8	12
1699	On the Origin of E-Selectivity in the Ring-Opening Metathesis Polymerization with Molybdenum Imido Alkylidene N-Heterocyclic Carbene Complexes. Organometallics, 2021, 40, 2478-2488.	1.1	6
1700	Unveiling Five Naked Structures of Tartaric Acid. Angewandte Chemie - International Edition, 2021, 60, 17410-17414.	7.2	10
1701	Influence of 5-Methylation and the 2′- and 3′-Hydroxy Substituents on the Base Pairing Energies of Protonated Cytidine Nucleoside Analogue Base Pairs: Implications for the Stabilities of <i>i</i> Motif Structures. Journal of Physical Chemistry A, 2021, 125, 5939-5955.	1.1	8
1702	A lead(II) toluene complex. Mendeleev Communications, 2021, 31, 471-474.	0.6	2
1703	Could London Dispersion Force Control Regioselective (2 + 2) Cyclodimerizations of Benzynes? YES: Application to the Synthesis of Helical Biphenylenes. Journal of the American Chemical Society, 2021, 143, 10853-10859.	6.6	19
1704	Group 12 Carbonates and their Binary Complexes with Nitrogen Bases and FH 2 Z Molecules (Z=P, As,) Tj ETQqO	0 0 rgBT /	Overlock 10
1705	Enhancing the absorption of 1-chloro-1,2,2,2-tetrafluoroethane on carbon nanotubes: an ab initio study. Bulletin of Materials Science, 2021, 44, 1.	0.8	31
1706	Synthesis of Nonaromatic Macromolecular Luminogens, DFT Studies on Photophysics, and Oâ€Đonor Selective Onâ^'Off Sensors: Contributions of In Situ <i>N</i> â€(Methylol)Acrylamido Comonomers. Advanced Optical Materials, 2021, 9, 2100802.	3.6	11
1708	Studies of Nature of Uncommon Bifurcated I–I···( <u>I</u> – <u>M</u> ) Metal-Involving Noncovalent Interaction in Palladium(II) and Platinum(II) Isocyanide Cocrystals. Inorganic Chemistry, 2021, 60, 13200-13211.	1.9	16
1709	Macrolactonization Reactions Driven by a Pentafluorobenzoyl Group**. Angewandte Chemie - International Edition, 2021, 60, 19843-19851.	7.2	6
1710	Charge Assisted S/Se Chalcogen Bonds in SAM Riboswitches: A Combined PDB and ab Initio Study. ACS Chemical Biology, 2021, 16, 1701-1708.	1.6	13

#	Article	IF	CITATIONS
1711	Hexaphenylditetrels – When Longer Bonds Provide Higher Stability. Chemistry - A European Journal, 2021, 27, 13699-13702.	1.7	9
1712	Atomic Clusters: Structure, Reactivity, Bonding, and Dynamics. Frontiers in Chemistry, 2021, 9, 730548.	1.8	14
1713	Diaryliodonium Tetrachloroplatinates(II): Recognition of a Trifurcated Metal-Involving μ <sub>3</sub> -I···(Cl,Cl,Pt) Halogen Bond. Crystal Growth and Design, 2021, 21, 5360-5372.	1.4	23
1714	DISPERSION-CORRECTED DENSITY FUNCTIONAL THEORY STUDIES ON GLYCOLIC ACID-METAL COMPLEXES. Journal of Structural Chemistry, 2021, 62, 1167-1183.	0.3	0
1715	Theoretical Exploration of Copper-Catalyzed Mechanisms of Cope-Type Hydroamination of Cyclopropene and Oxime. Journal of Organometallic Chemistry, 2021, 946-947, 121889.	0.8	0
1716	Role of β-CD Macromolecule Anchored to α-Fe <sub>2</sub> O <sub>3</sub> /TiO <sub>2</sub> on the Selectivity and Partial Oxidation of Guaiacol to Add-Value Products. ACS Sustainable Chemistry and Engineering, 2021, 9, 11427-11438.	3.2	4
1717	Spodium Bonds in Biological Systems: Expanding the Role of Zn in Protein Structure and Function. Journal of Chemical Information and Modeling, 2021, 61, 3945-3954.	2.5	21
1718	Computational Study of Homogeneous Multimetallic Cooperative Catalysis. Topics in Catalysis, 0, , 1.	1.3	11
1719	Insight into elastic anisotropy, mechanical and dynamical stability, electronic properties, bonding and weak interactions analysis of LuAuSn Half-Heusler. Solid State Sciences, 2021, 118, 106677.	1.5	17
1720	NCI: looking at solute/solvent interactions. Electronic Structure, 2021, 3, 034006.	1.0	1
1721	Computational investigation, comparative approaches, molecular structural, vibrational spectral, non-covalent interaction (NCI), and electron excitations analysis of benzodiazepine derivatives. Journal of Molecular Modeling, 2021, 27, 266.	0.8	13
1722	The effect of different substituent on ESIPT fluorescence features of 2-(2'-hydroxyphenyl)-4-chloro-methylthiazole derivatives: A DFT/TD-DFT study. Chinese Physics B, O, , .	0.7	0
1723	Theobroma cacao L. compounds: Theoretical study and molecular modeling as inhibitors of main SARS-CoV-2 protease. Biomedicine and Pharmacotherapy, 2021, 140, 111764.	2.5	17
1724	Uncovering the Activity of Alkaline Earth Metal Hydrogenation Catalysis Through Molecular Volcano Plots. Topics in Catalysis, 2022, 65, 289-295.	1.3	3
1725	Cis–trans isomerisation and absorption properties of the ring-extended azobenzene. Molecular Physics, 0, , Â.	0.8	0
1726	Removal of hydrogen sulfide from a binary mixture with methane gas, using IRMOF-1: a theoretical investigation. Journal of Molecular Modeling, 2021, 27, 240.	0.8	4
1727	Diethyl phenylphosphonite contributing to solid electrolyte interphase and cathode electrolyte interphase for lithium metal batteries. Journal of Energy Chemistry, 2021, 63, 566-573.	7.1	13
1728	Macrolactonization Reactions Driven by a Pentafluorobenzoyl Group**. Angewandte Chemie, 2021, 133, 19996-20004.	1.6	Ο

ARTICLE IF CITATIONS Mechanism and regio- and stereoselectivity in NHC-catalyzed reaction of 2-bromoenals with 1729 1.0 2 l²-ketoamides. Molecular Catalysis, 2021, 513, 111790. A comprehensive investigation of the intermolecular interactions between <u>CH<sub>2</sub>N<sub>2</u></sub>and X<sub>12</sub>Y<sub>12</sub>(X = B, Al, Ga; Y = N, P, As) nanocages. Canadian Journal of Chemistry, 2021, 99, 733-741. Transforming 3D CAUâ€10â€H into 2D Materials with High Base Stability for Membrane Separation. 1731 1.7 6 Chemistry - an Asian Journal, 2021, 16, 3236-3243. Halogen Interactions in Halogenated Oxindoles: Crystallographic and Computational Investigations of Intermolecular Interactions. Molecules, 2021, 26, 5487. Adsorption performance of boron nitride nanomaterials as effective drug delivery carriers for anticancer drugs based on density functional theory. Computational and Theoretical Chemistry, 2021, 1733 1.1 13 1203, 113360. Unravelling the Interactions of Magnetic Ionic Liquids by Energy Decomposition Schemes: Towards a Transferable Polarizable Force Field. Molecules, 2021, 26, 5526. 1.7 ï€â€"Ï€ Noncovalent Interaction Involving 1,2,4- and 1,3,4-Oxadiazole Systems: The Combined Experimental, 1735 1.7 32 Theoretical, and Database Study. Molecules, 2021, 26, 5672. Importance of Anionâ<sup>~</sup>ï€ Interactions in RNA GAAA and GGAG Tetraloops: A Combined MD and QM Study. 1736 2.3 Journal of Chemical Theory and Computation, 2021, 17, 6624-6633. Isomerization of Functionalized Olefins by Using the Dinuclear Catalyst 1737 [Pd<sup>l</sup>(<i>μ</i>â€Br)(P<sup><i>t</i>?sup>Bu<sub>3</sub>)]<sub>2</sub>: A Mechanistic Study. 1.7 5 Chemistry - A Euròpean Journal, 2021, 27, 15227-15239. Synthesis and Tetraphenylethylene-Based Aggregation-Induced Emission Probe for Rapid Detection of 1.6 Nitroaromatic Compounds in Áqueous Media. ACS Omega, 2021, 6, 25447-25460. Origin of the Rate Acceleration in the Câ<sup>^</sup>C Reductive Elimination from Pt(IV)â€complex in a [Ga<sub>4</sub>L<sub>6</sub>]<sup>12a^'</sup> Supramolecular Metallocage. Chemistry - A European 1739 9 1.7 Journal, 2021, 27, 15973-15980. A Comprehensive Picture of the Structures, Energies, and Bonding in the Alanine Dimers. 1740 1.0 ChemPhysChem, 2021, 22, 2401-2412. Distance Effects of Phenylpiperazine-Containing Methacrylic Polymers on Optical and Structural 1741 1.2 3 Properties. Journal of Physical Chemistry B, 2021, 125, 10629-10638. Solvent driven structural topologies involving unconventional O H(methanol)â<ï€ contact and anti-cooperative HBâ∢anion-Ï€â< HB assemblies with unusual enclathration of dual guest (H2O)4 cores in 1742 1.0 Mn(II) and Ni(II) coordination compounds: Antiproliferative evaluation and theoretical studies. Polyhedron, 2021, 210, 115503 Accelerated Dimerization of α,Î<sup>2</sup>-Unsaturated D-Xylo-Hexofurano-5-ulose Derivatives through 1743 1.7 0 Asynchronous Hetero-Diels–Alder Reaction. Journal of Organic Chemistry, 2021, 86, 12802-12812. Novel Oxidovanadium Complexes with Redox-Active R-Mian and R-Bian Ligands: Synthesis, Structure, 1744 Redox and Catalytic Properties. Molecules, 2021, 26, 5706. Novel Coordination Mode in the Potassium Mefenamate Trihydrate Polymeric Structure. Symmetry, 1745 1.1 0 2021, 13, 1761. Unconventional π-hole and Semi-coordination regium bonding interactions directed supramolecular 1746 assemblies in pyridinedicarboxylato bridged polymeric Cu(II) Compounds: Antiproliferative evaluation 1.2 and theoretical studies. Inorganica Chimica Acta, 2021, 525, 120461.

#	Article	IF	Citations
1747	Thermodynamics and Intermolecular Interactions during the Insertion of Anionic Naproxen into Model Cell Membranes. Journal of Physical Chemistry B, 2021, 125, 10383-10391.	1.2	13
1748	Structural, surface, and computational analysis of two vitamin-B1 crystals with sulfonimide-based anions. Zeitschrift Fur Kristallographie - Crystalline Materials, 2021, .	0.4	0
1749	A binuclear copper(II) complex based on hydrazone ligand: Characterization, molecular docking, and theoretical and antimicrobial investigation. Applied Organometallic Chemistry, 2022, 36, e6461.	1.7	7
1750	Adsorption of industrial dyes on functionalized and nonfunctionalized asphaltene: A combined molecular dynamics and quantum mechanics study. Journal of Molecular Liquids, 2021, 337, 116433.	2.3	20
1751	Importance of Van der Waals Interactions in Hydrogen Adsorption on a Silicon-carbide Nanotube Revisited with vdW-DFT and Quantum Monte Carlo. ACS Omega, 2021, 6, 24630-24636.	1.6	12
1752	Experimental and Theoretical Exploration of Volumetric Properties of Aminobutyric Acid and l-Valine in the Electrolytic Environment at T = 283.15 to 318.15 K and Pressure P = 0.1 MPa. Journal of Chemical & Engineering Data, 0, , .	1.0	0
1753	How Aromatic Fluorination Exchanges the Interaction Role of Pyridine with Carbonyl Compounds: The Formaldehyde Adduct. Chemistry - A European Journal, 2021, 27, 13870-13878.	1.7	6
1754	Enantioselectivity in Rutheniumâ€Catalyzed Propargylic Substitution Reactions of Propargylic Alcohols with Acetone: A DFT Study. Chemistry - an Asian Journal, 2021, 16, 3760-3766. Effect of Al- and Ga-doping on the adsorption of H <mml:math< td=""><td>1.7</td><td>5</td></mml:math<>	1.7	5
1755	xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:msub><mml:mrow /&gt;<mml:mn>2</mml:mn></mml:mrow </mml:msub> SiCl <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"&gt;<mml:msub><mml:mrow /&gt;<mml:mn>2</mml:mn></mml:mrow </mml:msub>onto the outer surface of boron nitride nanotube: a</mml:math 	0.2	12
1756	DFT study. Comptes Rendus Chimie, 2021, 24, 291-304. Diastereoselective Double Câ€H Functionalization of Chiral Ferrocenes with Heteroaromatics. Chemistry - A European Journal, 2021, 27, 15501-15507.	1.7	7
1757	Experimental and theoretical vibrational study of the fungicide pyraclostrobin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 259, 119888.	2.0	7
1758	An insight into the supramolecular interactions in two linear polyvanadates. Journal of Molecular Structure, 2021, 1242, 130681.	1.8	2
1759	First-principles characterisation of spectroscopic and bonding properties of cationic bismuth carbide clusters. Computational and Theoretical Chemistry, 2021, 1204, 113372.	1.1	0
1760	Vinyl chloride adsorption onto the surface of pristine, Al-, and Ga-doped boron nitride nanotube: A DFT study. Solid State Communications, 2021, 337, 114440.	0.9	28
1761	Structure and energetics of intermolecular association in two lurasidone co-amorphous drug systems. Journal of Molecular Structure, 2021, 1242, 130709.	1.8	4
1762	Adsorption of alkali and alkaline earth ions on nanocages using density functional theory. Computational and Theoretical Chemistry, 2021, 1204, 113391.	1.1	35
1763	Investigation of molecular interactions insight into some biologically active amino acids and aqueous solutions of an anti-malarial drug by physicochemical and theoretical approach. Journal of Molecular Liquids, 2021, 341, 116933.	2.3	20
1764	A rotational study of the 1:1 adduct of ethanol and 1,4-dioxane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 261, 120086.	2.0	2

#	Article	IF	CITATIONS
1765	Density functional theory-based analyses on selective gas separation by β-PVDF-supported ionic liquid membranes. Journal of Molecular Graphics and Modelling, 2021, 108, 108004.	1.3	2
1766	A combined experimental and theoretical analysis on the solid-state supramolecular assemblies of pent‑2-ynol derivatives. Journal of Molecular Structure, 2021, 1243, 130813.	1.8	4
1767	A DFT and molecular dynamics simulation study of single-walled carbon nanotube as a drug delivery system for few model nitrogen mustard drugs. Journal of Molecular Structure, 2021, 1243, 130877.	1.8	3
1768	Benzoato bridged dinuclear Mn(II) and Cu(II) compounds involving guest chlorobenzoates and dimeric paddle wheel supramolecular assemblies: Antiproliferative evaluation and theoretical studies. Polyhedron, 2021, 208, 115409.	1.0	9
1769	Catalyzed stereo-selective hydrogenation of ynamides to give enamines: Ethanol as a hydrogen donor. Journal of Organometallic Chemistry, 2021, 952, 122024.	0.8	2
1770	Experimental and computational structural studies of 5-substituted-3-(1-arylmethyl-1,2,3,6-tetrahydropyridin-4-yl)-1H-indoles. Journal of Molecular Structure, 2021, 1245, 130998.	1.8	2
1771	Nicotinamide-based supergelator self-assembling via asymmetric hydrogen bonding NH⋯OC and H⋯Brâ^' pattern for reusable, moldable and self-healable nontoxic fuel gels. Journal of Colloid and Interface Science, 2021, 603, 182-190.	5.0	3
1772	Experimental and theoretical investigation of synthesized pregnenolone derivatives via palladium catalyzed cross coupling reactions, their anticancer activity against lung cancer cells. Journal of Molecular Structure, 2021, 1245, 131115.	1.8	7
1773	Chirality, structure and hydrogen bonding in dithiols: Rotational spectrum of the chiral and meso 2,3-butanedithiol. Journal of Molecular Structure, 2021, 1246, 131221.	1.8	1
1774	Crystal structure, IR investigation and interpretation of interactions in cobalt selenate pentahydrate. Chemical Data Collections, 2021, 36, 100776.	1.1	Ο
1775	Recognition and visual detection of ADP and ATP based on a dinuclear Zn(II)-complex with pyrocatechol violet in water. Dyes and Pigments, 2021, 196, 109827.	2.0	2
1776	Solvothermal self assembly of three lanthanide(III)-succinates: Crystal structure, topological analysis and DFT calculations on water channel. Journal of Molecular Structure, 2021, 1245, 131094.	1.8	12
1777	Supramolecular, spectroscopic and computational analysis of weak interactions in some thiosemicarbazones derived from 5-acetylbarbituric acid. Journal of Molecular Structure, 2021, 1245, 131031.	1.8	1
1778	Unconventional enclathration of guest adipic acid and energetically significant antiparallel π-stacked ternary assemblies involving unusual regium-π(chelate) contacts in phenanthroline-based Ni(II) and Cu(II) compounds—Antiproliferative evaluation and theoretical studies. Journal of Molecular Structure, 2021, 1245, 131038.	1.8	8
1779	Binding of vanadium ions and complexes to proteins and enzymes in aqueous solution. Coordination Chemistry Reviews, 2021, 449, 214192.	9.5	40
1780	Metalloid Chalcogen–pnictogen Ï <i>f</i> -hole bonding competition in stibanyl telluranes. Journal of Organometallic Chemistry, 2021, 954-955, 122092.	0.8	5
1781	Face specific doping of Janus all-cis-1,2,3,4,5,6-hexafluorocyclohexane with superalkalis and alkaline earth metals leads to enhanced static and dynamic NLO responses. Journal of Physics and Chemistry of Solids, 2022, 160, 110361.	1.9	22
1782	Effectively controlling the ESIPT behavior and fluorescence feature of 2-(2′-hydroxyphenyl)-4-chloromethylthiazole by changing its π-conjugation: A theoretical exploration. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 422, 113548.	2.0	9

	CITATION REPORT		
ARTICLE Phenanthroline-based Ni(II) coordination compounds involving unconventional discrete		IF	CITATIONS
fumarate-water-nitrate clusters and energetically significant cooperative ternary i€-stacked assemblies: Antiproliferative evaluation and theoretical studies. Journal of Molecular Structu 2022, 1248, 131424.	ure,	1.8	10
Encapsulated hydroxychloroquine and chloroquine into cyclic oligosaccharides are the pote therapeutics for COVID-19: insights from first-principles calculations. Journal of Molecular Structure, 2022, 1247, 131371.	ential	1.8	12
Significant bonding rearrangements triggered by Mg4 clusters. Journal of Chemical Physics, 044302.	, 2021, 154,	1.2	2
Adsorption of 1-chloro-1,2,2,2-tetrafluoroethane on pristine, Al, Ga-doped boron nitride nar study involving PBC-DFT, NBO analysis, and QTAIM. Canadian Journal of Chemistry, 2021, 9	notubes: a 99, 51-62.	0.6	27
Non-covalent interactions involving remote substituents influence the topologies of supran chains featuring hydroxyl-O–Hâ <o(hydroxyl) bonding="" crystals="" hydrogen="" in="" of<br="">(HOCH2CH2)2NC()N(H)(C6H4Y-4) for Y = H, Me, Cl and NO2. CrystEngComm, 2021, 23</o(hydroxyl)>		1.3	6
Luminescent cyclometalated platinum( <scp>ii</scp> ) complexes with acyclic diaminocarbe structural, photophysical and biological properties. Dalton Transactions, 2021, 50, 4539-45	ne ligands: 554.	1.6	25
Selenium chalcogen bonds are involved in protein–carbohydrate recognition: a combinec theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 17656-17662.	l PDB and	1.3	14
A dynamic picture of the halolactonization reaction through a combination of <i>ab initio&lt; metadynamics and experimental investigations. Chemical Science, 2021, 12, 7746-7757.</i>	/i>	3.7	10
Mechanism of iron complexes catalyzed in the <i>N</i> -formylation of amines with CO <sub and H<sub>2</sub>: the superior performance of N<math>\hat{a}\in</math>"H ligand methylated complexes. Phy Chemistry Chemical Physics, 2021, 23, 16675-16689.</sub 	⊃>2 ∕sical	1.3	3
Yet another perspective on hole interactions. Physical Chemistry Chemical Physics, 2021, 2 19948-19963.	3,	1.3	23
Biologically relevant unusual cooperative assemblies and fascinating infinite crown-like supramolecular nitrate–water hosts involving guest complex cations in bipyridine and phenanthroline-based Cu( <scp>ii</scp> ) coordination compounds: antiproliferative evaluat theoretical studies. New Journal of Chemistry, 2021, 45, 8269-8282.	tion and	1.4	14
Computational and infrared spectroscopic investigations of N-substituted carbazoles. Phys Chemistry Chemical Physics, 2021, 23, 8426-8438.	ical	1.3	0
Host guest chemistry and supramolecular doping in triphenylamine-based covalent framew Au(111). Nanoscale, 2021, 13, 9798-9807.	orks on	2.8	5
Nature and strength of intrinsic cation–anion interactions of 1-alkyl-3-methylimidazolium hexafluorophosphate clusters. Physical Chemistry Chemical Physics, 2021, 23, 13405-1341	.8.	1.3	3
Electron belt-to-Ïf-hole switch of noncovalently bound iodine( <scp>i</scp> ) atoms in dithic metal complexes. Inorganic Chemistry Frontiers, 2021, 8, 2505-2517.	ocarbamate	3.0	25
The origin of the regiospecificity of acrolein dimerization. RSC Advances, 2021, 11, 7459-74	465.	1.7	1

1799	Mechanistic insights into rhodium-catalyzed enantioselective allylic alkylation for quaternary stereogenic centers. Chemical Science, 2021, 12, 2527-2539.	3.7	9
1800	Dispersion forces drive water oxidation in molecular ruthenium catalysts. RSC Advances, 2021, 11, 425-432.	1.7	4

#

1783

1785

1787

1789

1791

1792

1793

1795

1797

#	Article	IF	CITATIONS
1801	Supramolecular network of a framework material supported by the anion–π linkage of Keggin-type heteropolyoxotungstates: experimental and theoretical insights. Dalton Transactions, 2021, 50, 1895-1900.	1.6	31
1802	A molecular twist on hydrophobicity. Chemical Science, 2021, 12, 9233-9245.	3.7	22
1803	Computational prediction of the supramolecular self-assembling properties of organic molecules: the role of conformational flexibility of amide moieties. Physical Chemistry Chemical Physics, 2021, 23, 20453-20465.	1.3	2
1804	Unprecedented copper(ii) coordination induced nucleophilic cleavage of a quinoxaline heterocycle: structural and computational studies. CrystEngComm, 2021, 23, 5078-5086.	1.3	3
1805	Unveiling the regioselectivity in electrophilic aromatic substitution reactions of deactivated benzenes through molecular electron density theory. New Journal of Chemistry, 2021, 45, 13626-13638.	1.4	10
1806	Change in molecular shapes of the trinuclear Cull2ZnII complexes on Schiff base reduction: structural and theoretical investigations. CrystEngComm, 2021, 23, 4848-4856.	1.3	3
1807	Synthesis and crystal structure of the simultaneous binding of Ni( <scp>ii</scp> ) cation and chloride by the protonated 2,4,6 tris-(2-pyridyl)-1,3,5 triazine ligand: theoretical investigations of anionâ<ï€, ï€â<ï€ and hydrogen bonding interactions. New Journal of Chemistry, 2021, 45, 11689-11696.	1.4	13
1808	On the nature of recurrent Auâ<ï€ motifs in tris(2,2′-bipyridine)M( <scp>ii</scp> ) (M = Fe, Co and Ni) dicyanoaurate( <scp>i</scp> ) salts: X-ray analysis and theoretical rationalization. Dalton Transactions, 2021, 50, 16954-16960.	1.6	4
1809	Understanding the planar conformations in diarylsubstituted heteroarenes: structural and theoretical insights. CrystEngComm, 2021, 23, 3144-3151.	1.3	7
1810	Impact of van der Waals interactions on the structural and nonlinear optical properties of azobenzene switches. Physical Chemistry Chemical Physics, 2021, 23, 21227-21239.	1.3	14
1811	Integrated experimental/computational approaches to characterize the systems formed by vanadium with proteins and enzymes. Inorganic Chemistry Frontiers, 2021, 8, 1951-1974.	3.0	24
1812	On the question of steric repulsion <i>versus</i> noncovalent attractive interactions in chiral phosphoric acid catalyzed asymmetric reactions. Physical Chemistry Chemical Physics, 2021, 23, 18936-18950.	1.3	10
1813	Coupling Reactions of Alkynyl Indoles and CO <sub>2</sub> by Bicyclic Guanidine: Origin of Catalytic Activity?. Chemistry - an Asian Journal, 2017, 12, 1780-1789.	1.7	16
1814	Interaction of the nitrosyl ruthenium complex [Ru <sup>II</sup> (NH.NHqâ€R)(tpy)NO] <sup>3+</sup> with human serum albumin: a spectroscopic and computational investigation. Luminescence, 2021, 36, 391-408.	1.5	7
1815	Sensing of toxic Lewisite (L <sub>1</sub> , L <sub>2</sub> , and L <sub>3</sub> ) molecules by graphdiyne nanoflake using density functional theory calculations and quantum theory of atoms in molecule analysis. Journal of Physical Organic Chemistry, 2021, 34, e4181.	0.9	18
1816	Recognition of anions using urea and thiourea substituted calixarenes: A density functional theory study of non-covalent interactions. Chemical Physics, 2018, 501, 68-77.	0.9	20
1817	Exploring the physicochemical properties of para-xylyl linked DBU-based dicationic ionic liquids consist of various anions: A GD3–M06–2X study. Journal of Molecular Liquids, 2020, 310, 113060.	2.3	8
1818	Carbon nitride 2-D surface as a highly selective electrochemical sensor for V-series nerve agents. Journal of Molecular Liquids, 2020, 311, 113357.	2.3	38

#	Article	IF	CITATIONS
1819	Synthesis, crystal structure, catalytic and anti-Trypanosoma cruzi activity of a new chromium(III) complex containing bis(3,5-dimethylpyrazol-1-yl)methane. Journal of Molecular Structure, 2017, 1146, 365-372.	1.8	14
1820	Quantitative insights into the crystal structure of a mixed-ligand Co(III) complex: Experimental and theoretical studies. Journal of Molecular Structure, 2020, 1216, 128207.	1.8	19
1821	Halogen Bonding Involving Palladium(II) as an XB Acceptor. Crystal Growth and Design, 2021, 21, 1159-1177.	1.4	25
1822	Stereoselective Reductions of 3-Substituted Cyclobutanones: A Comparison between Experiment and Theory. Journal of Organic Chemistry, 2020, 85, 7803-7816.	1.7	5
1823	Intramolecular Dispersion Attraction in Tetraalkylammonium Cations Revealed by Cryogenic Ion Mobility Mass Spectrometry. Journal of Physical Chemistry A, 2020, 124, 7999-8004.	1,1	10
1824	Lactic Acid Spectroscopy: Intra- and Intermolecular Interactions. Journal of Physical Chemistry A, 2021, 125, 218-229.	1.1	7
1825	Importance of C–H Hydrogen Bonding in Asymmetric Catalysis. RSC Catalysis Series, 2019, , 26-65.	0.1	1
1826	Analysis of Reactivity from the Noncovalent Interactions Perspective. RSC Catalysis Series, 2019, , 628-643.	0.1	2
1827	Computational design of <i>p</i> -(dimethylamino)benzylidene-derived push–pull polyenes with high first-hyperpolarizabilities. Physical Chemistry Chemical Physics, 2020, 22, 5090-5104.	1.3	7
1828	Reinterpreting π-stacking. Physical Chemistry Chemical Physics, 2020, 22, 24870-24886.	1.3	62
1829	A resorcinarene-based tetrabenzoimidazolylidene complex of rhodium. Dalton Transactions, 2020, 49, 3181-3186.	1.6	2
1830	On the importance of ï€-hole spodium bonding in tricoordinated Hg <sup>II</sup> complexes. Dalton Transactions, 2020, 49, 17547-17551.	1.6	25
1831	Learning on-top: Regressing the on-top pair density for real-space visualization of electron correlation. Journal of Chemical Physics, 2020, 153, 204111.	1.2	10
1832	Distinguishing between chemical bonding and physical binding using electron localization function (ELF). Journal of Physics Condensed Matter, 2020, 32, 315502.	0.7	137
1833	Subatomic resolution X-ray structures of green fluorescent protein. IUCrJ, 2019, 6, 387-400.	1.0	24
1834	Intra- and intermolecular interactions in a series of chlorido-tricarbonyl-diazabutadienerhenium(I) complexes: structural and theoretical studies. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 417-426.	0.5	3
1835	2-[(4-Chlorophenyl)sulfanyl]-2-methoxy-1-phenylethan-1-one: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 703-708.	0.2	2
1836	4-(4-Acetyl-5-methyl-1H-1,2,3-triazol-1-yl)benzonitrile: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1195-1200.	0.2	6

#	Article	IF	CITATIONS
1837	Utilizing Hirshfeld surface calculations, non-covalent interaction (NCI) plots and the calculation of interaction energies in the analysis of molecular packing. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 308-318.	0.2	354
1838	3,3-Bis(2-hydroxyethyl)-1-(4-methylbenzoyl)thiourea: crystal structure, Hirshfeld surface analysis and computational study. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1472-1478.	0.2	6
1839	3,3-Bis(2-hydroxyethyl)-1-(4-nitrobenzoyl)thiourea: crystal structure, Hirshfeld surface analysis and computational study. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 155-161.	0.2	6
1840	Crystal structure and Hirshfeld surface analysis of the product of the ring-opening reaction of a dihydrobenzoxazine: 6,6′-[(cyclohexylazanediyl)bis(methylene)]bis(2,4-dimethylphenol). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1239-1244.	0.2	3
1841	ALKBH7 Variant Related to Prostate Cancer Exhibits Altered Substrate Binding. PLoS Computational Biology, 2017, 13, e1005345.	1.5	24
1842	The mechanism of dissociation of cytosine pairs mediated by silver ions. Computer Research and Modeling, 2019, 11, 685-693.	0.2	1
1845	Perspective: Chemical Information Encoded in Electron Density. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2018, 34, 567-580.	2.2	4
1846	TrialkylsulfoniumÂand TetraalkylammoniumÂSalts as Hydrogen-Bonding Catalysts in an Aza-Diels-Alder Reaction: Experimental and Computational Studies. Heterocycles, 2020, 101, 580.	0.4	10
1847	Photoinduced electron transfer in non-covalent complexes of C60 and phosphangulene oxide derivatives. Dalton Transactions, 2021, 50, 16214-16222.	1.6	3
1848	Coordination <i>versus</i> spodium bonds in dinuclear Zn( <scp>ii</scp> ) and Cd( <scp>ii</scp> ) complexes with a dithiophosphate ligand. New Journal of Chemistry, 2021, 45, 19402-19415.	1.4	17
1849	Modified-amino acid/peptide pyrimidine analogs: synthesis, structural characterization and DFT studies of N-(pyrimidyl)gabapentine and N-(pyrimidyl)baclofen. New Journal of Chemistry, 0, , .	1.4	1
1850	Lead( <scp>ii</scp> ) supramolecular structures formed through a cooperative influence of the hydrazinecarbothioamide derived and ancillary ligands. CrystEngComm, 2022, 24, 368-378.	1.3	7
1851	Influence of non-covalent interactions in dictating the polarity and mobility of charge carriers in a series of crystalline NDIs: a computational case study. RSC Advances, 2021, 11, 33703-33713.	1.7	8
1852	Theoretical Investigation of Excited-State Intramolecular Double-Proton Transfer Mechanism of Substituent Modified 1, 3-Bis (2-Pyridylimino)-4,7-Dihydroxyisoindole in Dichloromethane Solution. Journal of Computational Biophysics and Chemistry, 2021, 20, 707-718.	1.0	5
1853	Stacked but not Stuck: Unveiling the Role of π→π* Interactions with the Help of the Benzofuran–Formaldehyde Complex. Angewandte Chemie - International Edition, 2022, 61, .	7.2	15
1854	Ab initio investigation for the adsorption of acrolein onto the surface of C60, C59Si, and C59Ge: NBO, QTAIM, and NCI analyses. Structural Chemistry, 2022, 33, 363-378.	1.0	26
1855	Contrasting the Mechanism of H <sub>2</sub> Activation by Monomeric and Potassiumâ€6tabilized Dimeric Al <sup>I</sup> Complexes: Do Potassium Atoms Exert any Cooperative Effect?. Chemistry - A European Journal, 2021, 27, 17369-17378.	1.7	9
1856	Nazarov Cyclizations Catalyzed by BINOL Phosphoric Acid Derivatives: Quantum Chemistry Struggles To Predict the Enantioselectivity. Journal of Organic Chemistry, 2022, 87, 1710-1722.	1.7	5

#	Article	IF	CITATIONS
1857	Solid State Characterization of One―and Twoâ€Electron Oxidized Cu <sup>II</sup> â€salen Complexes with <i>para</i> ‣ubstituents: Geometric Structureâ€Magnetic Property Relationship. European Journal of Inorganic Chemistry, 2021, 2021, 4133-4145.	1.0	5
1858	Insights into Organoamine-Catalyzed Asymmetric Synthesis of Axially Chiral Allenoates Using Morita–Baylis–Hillman Carbonates and Trisubstituted Allenoates: Mechanism and Origin of Stereoselectivity. Journal of Organic Chemistry, 2021, 86, 15276-15283.	1.7	10
1859	A unified molecularâ€wide and electron density based concept of chemical bonding. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	6
1860	Noncovalent Interactions in Organometallic Chemistry: From Cohesion to Reactivity, a New Chapter. Accounts of Chemical Research, 2021, 54, 3828-3840.	7.6	22
1861	Intermolecular Interactions between Serine and C60, C59Si, and C59Ge: a DFT Study. Silicon, 2022, 14, 6075-6088.	1.8	27
1862	DFT Study for Adsorbing of Bromine Monochloride onto BNNT (5,5), BNNT (7,0), BC <sub>2</sub> NNT (5,5), and BC <sub>2</sub> NNT (7,0). Journal of Computational Biophysics and Chemistry, 2021, 20, 765-783.	1.0	35
1863	Theoretical Study of N-Heterocyclic-Carbene–ZnX2 (X = H, Me, Et) Complexes. Materials, 2021, 14, 6147.	1.3	12
1864	Stacked but not Stuck: Unveiling the Role of π → π* Interactions with the Help of the Benzofuranâ€Formaldehyde Complex. Angewandte Chemie, 2022, 134, e202113737.	1.6	2
1865	Alkylated Benzodithienoquinolizinium Salts as Possible Non-Fullerene Organic N-Type Semiconductors: An Experimental and Theoretical Study. Materials, 2021, 14, 6239.	1.3	0
1866	Bonding and Reactivity of a Pair of Neutral and Cationic Heterobimetallic RuZn2 Complexes. Inorganic Chemistry, 2021, 60, 16256-16265.	1.9	7
1867	Sizeâ€Induced Inversion of Selectivity in the Acylation of 1,2â€Diols. Chemistry - A European Journal, 2021, 27, 18084-18092.	1.7	3
1868	Univariate classification of phosphine ligation state and reactivity in cross-coupling catalysis. Science, 2021, 374, 301-308.	6.0	97
1869	Insights into the origin of selectivity for [2+2] cycloaddition step reaction involved in the mechanism of enantioselective reduction of ketones with borane catalyzed by a B-methoxy oxazaborolidine catalyst derived from (–)-β-pinene: an HMDFT and combined topological ELF, NCI and QTAIM study. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	1
1870	Computational chemistry methods for modelling non-covalent interactions and chemical reactivity— An overview. Journal of the Indian Chemical Society, 2021, 98, 100208.	1.3	22
1872	Noncovalent Interactions in Ionic Liquids. RSC Catalysis Series, 2019, , 350-376.	0.1	0
1873	Noncovalent Interactions in Biocatalysis – A Theoretical Perspective. RSC Catalysis Series, 2019, , 608-627.	0.1	0
1874	Computational asymmetric catalysis: On the origin of stereoselectivity in catalytic reactions. Advances in Physical Organic Chemistry, 2019, 53, 1-27.	0.5	2
1875	2-[(4-Bromophenyl)sulfanyl]-2-methoxy-1-phenylethan-1-one: crystal structure, Hirshfeld surface analysis and computational chemistry. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 816-822.	0.2	0

ARTICLE IF CITATIONS # 2-Methyl-4-(4-nitrophenyl)but-3-yn-2-ol: crystal structure, Hirshfeld surface analysis and computational chemistry study. Acta Crystallographica Section E: Crystallographic Communications, 1877 0.2 2 2019, 75, 1232-1238. <i>N</i>-Tosyl-<scp>L</scp>-proline benzene hemisolvate: a rare example of a hydrogen-bonded carboxylic acid dimer with symmetrically disordered H atoms. Acta Crystallographica Section C, 1878 0.2 Structural Chemistry, 2019, 75, 1228-1233. Anagostic Interactions in Alkyl-Fluorenyl-Substituted Nâ€Heterocyclic Carbene Complexes of 1879 0 0.5Palladium(II). Australian Journal of Chemistry, 2020, 73, 579. Crystal structure, Hirshfeld surface analysis and computational study of the 1:2 co-crystal formed between <i>N</i>,<i>N</i>,i>R</i>,i>ê $e^2$ -bis(pyridin-4-ylmethyl)ethanediamide and 4-chlorobenzoic acid. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 245-253. 0.2 1-Ethyl 2-methyl 3,4-bis(acetyloxy)pyrrolidine-1,2-dicarboxylate: crystal structure, Hirshfeld surface analysis and computational chemistry. Acta Crystallographica Section E: Crystallographic 1881 0.2 4 Communications, 2020, 76, 967-972.  $2,2\hat{a}\in^2$ -(Disulfanediyl)dibenzoic acid <i>N</i>,<i>N</i>dimethylformamide monosolvate: crystal structure, Hirsheld surface analysis and computational study. Acta Crystallographica Section E: 1882 0.2 Crystallographic Communications, 2020, 76, 1150-1157. 4-[(1<i>E</i>)-({[(Benzylsulfanyl)methanethioyl]amino}imino)methyl]benzene-1,3-diol chloroform 1883 hemisolvate: crystal structure, Hirshfeld surface analysis and computational study. Acta 0.2 0 Crystallographica Section E: Crystallographic Communications, 2020, 76, 990-997. 4-Nitrobenzyl 3,4-bis(acetyloxy)-2-(4-methoxyphenyl)pyrrolidine-1-carboxylate: crystal structure, Hirshfeld surface analysis and computational chemistry. Acta Crystallographica Section E: 1884 0.2 Crystallographic Communications, 2020, 76, 1080-1086. Decarbonylative Fluoroalkylation at Palladium(II): From Fundamental Organometallic Studies to 1885 25 6.6 Catalysis. Journal of the American Chemical Society, 2021, 143, 18617-18625. Studies of Catalyst-Controlled Regioselective Acetalization and Its Application to Single-Pot Synthesis of Differentially Protected Saccharides. Journal of the American Chemical Society, 2021, 143, 6.6 18592-18604. Chemical reactivity and binding interactions in ribonucleic acid<scp>â€</scp>peptide complexes. 1887 0 1.5 Proteins: Structure, Function and Bioinformatics, 2022, 90, 765-775. Removal of nafcillin sodium monohydrate from aqueous solution by hydrogels containing 1888 2.3 nanocellulose: An experimental and theoretical study. Journal of Mólecular Liquids, 2022, 347, 117946. Non-covalent interactions of cysteine onto C60, C59Si, and C59Ge: a DFT study. Journal of Molecular 1889 0.8 20 Modeling, 2021, 27, 330. Non-covalent interactions in hexanuclear polyoxidometalates [VIV6B20O50H8]8-. An experimental and theoretical approach. Polyhedron, 2021, 211, 115553. 1890 1.0 Chalcogen Bond Involving Zinc(II)/Cadmium(II) Carbonate and Its Enhancement by Spodium Bond. 1891 1.7 6 Molecules, 2021, 26, 6443. Tuneable separation of gold by selective precipitation using a simple and recyclable diamide. Nature 1892 5.8 36 Communications, 2021, 12, 6258. Spectroscopic Signatures of Hydrogen-Bonding Motifs in Protonic Ionic Liquid Systems: Insights from Diethylammonium Nitrate in the Solid State. Journal of Physical Chemistry C, 2021, 125, 24463-24476. 1893 1.54 Fluorinated dihydropyridines as candidates to block L-type voltage-dependent calcium channels. 1894 Journal of Biomolecular Structure and Dynamics, 2021, , 1-16.

#	Article	IF	CITATIONS
1895	Novel â€~main-part' isostructuralism in metal complexes with 1-methylimidazole: crystal structures, energy calculations and magnetic properties. Dalton Transactions, 2021, 50, 17029-17040.	1.6	1
1896	Molecular insights into the selective binding mechanism targeting parallel human telomeric G-quadruplex. Journal of Molecular Graphics and Modelling, 2022, 110, 108058.	1.3	8
1897	Molecular modeling of methacrylic composite materials doped with nonlinear optical azochromophores with various acceptor fragments. Computational Materials Science, 2022, 201, 110909.	1.4	2
1898	Combined gas-phase electron diffraction and coupled cluster determination of the molecular structure of 3,4-dinitrofurazan - A propellant ingredient. Journal of Molecular Structure, 2022, 1250, 131669.	1.8	2
1899	Micro-phase separation promoted by electrostatic field in electrospinning of alkaline polymer electrolytes: DFT and MD simulations. Chemical Engineering Science, 2022, 248, 117171.	1.9	9
1900	An ionic hydrogel with stimuli-responsive, self-healable and injectable characteristics for the targeted and sustained delivery of doxorubicin in the treatment of breast cancer. Materials Advances, 2022, 3, 632-646.	2.6	13
1901	Chapter 3. Theoretical Approaches. RSC Theoretical and Computational Chemistry Series, 2020, , 99-224.	0.7	1
1902	Chapter 9. Remarks and Conclusions. RSC Theoretical and Computational Chemistry Series, 2020, , 441-452.	0.7	0
1903	Arylhydrazones of α-keto esters via methanolysis of dichlorodiazabutadienes: synthesis and structural study. Mendeleev Communications, 2021, 31, 677-679.	0.6	8
1904	Photo-Triggered Chiroptical Switching of Platinum Complexes Bearing Azobenzene Moieties. Organometallics, 2021, 40, 3550-3559.	1.1	2
1905	Adsorption of acetic acid and benzoic acid on pristine and defect containing graphene: A DFT study. Computational and Theoretical Chemistry, 2022, 1207, 113504.	1.1	2
1906	Tris(6-diphenylphosphinoacenaphth-5-yl)gallium: Z-Type Ligand and Transmetalation Reagent. Organometallics, 2021, 40, 3785-3796.	1.1	3
1907	Charge Assisted Hydrogen Bonded Assemblies and Unconventional Oâ^™â^™â^™O Dichalcogen Bonding Interactions in Pyrazole-Based Isostructural Ni(II) and Mn(II) Compounds involving Anthraquinone Disulfonate: Antiproliferative Evaluation and Theoretical Studies. Journal of Molecular Structure, 2021, 1250, 131883.	1.8	6
1908	Novel microporous B6N6 covalent organic framework (COF) as an electrochemical sensor for the ultra-selective detection of nitroaniline isomers; a DFT outcome. Surfaces and Interfaces, 2021, 27, 101587.	1.5	14
1909	A Data-Driven Approach to the Development and Understanding of Chiroptical Sensors for Alcohols with Remote Î <sup>3</sup> -Stereocenters. Journal of the American Chemical Society, 2021, 143, 19187-19198.	6.6	12
1910	Complementary amide-based donor–acceptor with unique nano-scale aggregation, fluorescence, and band gap-lowering properties: a WORM memory device. Nanotechnology, 2021, 32, 025208.	1.3	7
1911	Crystalline assembly of perylene in metal–organic framework thin film: J-aggregate or excimer? Insight into the electronic structure. Journal of Physics Condensed Matter, 2021, 33, 034001.	0.7	1
1912	Design, Synthesis, and Application of Multiboron Heterocycle to Direct Amidation Catalyst. Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry, 2020, 78, 971-978.	0.0	3

#	Article	IF	CITATIONS
1913	A Computational Study on the Intramolecular C4-C8′ Interflavan Bond Formations of Tethered Catechin Derivatives. Bulletin of the Chemical Society of Japan, 2020, 93, 1107-1113.	2.0	1
1914	Die größenbeschleunigte kinetische Racematspaltung sekundär Alkohole. Angewandte Chemie, 2021, 133, 786-791.	1.6	4
1915	Study of Donor–Acceptor Bonds on the N â€Coordinated Sn/Pb(II) Atoms in peri â€Substituted Naphthalenes: Evidence of Pb→B Interaction. European Journal of Inorganic Chemistry, 2020, 2020, 3644-3653.	1.0	7
1916	Insights into conformational changes in AlkD bound to DNA with a yatakemycin adduct from computational simulations. Theoretical Chemistry Accounts, 2018, 137, .	0.5	0
1917	Towards a predictive model for polymer solubility using the noncovalent interaction index: polyethylene as a case study. Physical Chemistry Chemical Physics, 2021, 23, 25374-25387.	1.3	6
1918	Tyrosine-based photoluminescent diketopiperazine supramolecular aggregates. Soft Matter, 2021, 18, 137-145.	1.2	2
1919	Luminescent 2-phenylbenzothiazole cyclometalated Pt <sup>II</sup> and Ir <sup>III</sup> complexes with chelating P^O ligands. Dalton Transactions, 2021, 51, 274-285.	1.6	7
1920	A comparative study of noncovalent interactions in various Ni-compounds containing nitrogen heteroaromatic ligands and pseudohalides: A combined experimental and theoretical studies. Inorganica Chimica Acta, 2022, 531, 120702.	1.2	0
1921	Covalent triazine framework (CTF-0) surface as a smart sensing material for the detection of CWAs and industrial pollutants. Materials Science in Semiconductor Processing, 2022, 139, 106334.	1.9	21
1922	Computational Study of Mechanism and Enantioselectivity of Imine Reductase from <i>Amycolatopsis orientalis</i> . ChemistryOpen, 2022, 11, e202100250.	0.9	7
1923	Theoretical Aspects of Nonconventional Hydrogen Bonds in the Complexes of Aldehydes and Hydrogen Chalcogenides. Journal of Physical Chemistry A, 2021, 125, 10291-10302.	1.1	2
1924	London Dispersion Helps Refine Steric A-Values: Dispersion Energy Donor Scales. Journal of the American Chemical Society, 2021, 143, 20837-20848.	6.6	35
1925	To be or not to be? that is the entropic, enthalpic, and molecular interaction dilemma in the formation of (water)20 clusters and methane clathrate. ChemPhysChem, 2021, , .	1.0	4
1926	Synthesis, Structures, and Properties of Helically Fused Anthraquinones with Unusually Close Carbonyl arbonyl Contacts. Chemistry - A European Journal, 2021, , .	1.7	3
1927	The influence of secondary interactions on the [Ni(O2)]+ mediated aldehyde oxidation reactions. Journal of Inorganic Biochemistry, 2021, 227, 111668.	1.5	2
1928	Ïfâ€Hole Interactions of Tetrahedral Group IV–VIII Lewis Acid Centers with Lewis Bases: A Comparative Study. ChemistrySelect, 2021, 6, 11856-11864.	0.7	5
1929	Revealing the Structure and Noncovalent Interactions of Isolated Molecules by Laser-Desorption/Ionization-Loss Stimulated Raman Spectroscopy and Quantum Calculations. Journal of Physical Chemistry Letters, 2021, 12, 11273-11279.	2.1	3
1930	Energetic features of antiparallel stacking and hydrogen bonding interactions in two coordination complexes bearing 1,10-phenanthroline-2,9-dicarboxylic acid. Journal of Molecular Structure, 2022, 1251, 131963.	1.8	3

#	Article	IF	CITATIONS
1931	Pincer iridium(III)-catalyzed enantioselective C(sp3)-H functionalization via carbenoid C H insertion of 3-diazooxindoles with 1,4-cyclohexadiene. Chinese Chemical Letters, 2022, 33, 2437-2441.	4.8	7
1932	On the Importance of Halogen Bonding Interactions in Two X-ray Structures Containing All Four (F,) Tj ETQq1 1	0.784314 1.0	rgBT/Overlo
1933	Cluster Assembled Silicon-Lithium Nanostructures: A Nanowire Confined Inside a Carbon Nanotube. Frontiers in Chemistry, 2021, 9, 767421.	1.8	1
1934	Helium nanodroplet infrared spectroscopy of oxazole-(water)n (n = 1,2) clusters. AIP Advances, 2021, 11, 115112.	0.6	0
1935	Novel and Polynuclear K- and Na-Based Superalkali Hydroxides as Superbases Better Than Li-Related Species and Their Enhanced Properties: An Ab Initio Exploration. ACS Omega, 2021, 6, 31077-31092.	1.6	9
1936	Spectroscopic/Computational Characterization and the X-ray Structure of the Adduct of the V <sup>N</sup>	1.9	12
1937	Interactions of Urea-Based Inhibitors with Prostate-Specific Membrane Antigen for Boron Neutron Capture Therapy. ACS Omega, 2021, 6, 33354-33369.	1.6	2
1938	Azaâ€Dielsâ€Alder Reaction of Danishefsky's Diene with Imine Catalyzed by Nâ€Heterocyclic Imidazole Halogen Bond Donors. ChemistrySelect, 2021, 6, 12843-12851.	0.7	6
1939	Janusene as a Silver Ion Scavenger: Insights from Computation. New Journal of Chemistry, 0, , .	1.4	1
1940	Computational insights into metal-catalyzed asymmetric hydrogenation. Advances in Catalysis, 2021, 68, 385-426.	0.1	1
1941	Supramolecular Approach to Tuning the Photophysical Properties of Quadrupolar Squaraines. Frontiers in Chemistry, 2021, 9, 800541.	1.8	1
1942	Theoretical reconsideration of the mechanism of the excited state proton transfer of indigo carmine in water. Journal of Molecular Liquids, 2022, 347, 118365.	2.3	15
1943	Synthesis, structural topologies and anticancer evaluation of phenanthroline-based 2,6-pyridinedicarboxylato Cu(II) and Ni(II) compounds. Polyhedron, 2022, 213, 115632.	1.0	6
1944	Chemical bonding, magnetic and electronic properties, mechanical and dynamical stabilities of DyOs4P12 filled-skutterudite: DFT and QTAIM insight. Materials Chemistry and Physics, 2022, 278, 125684.	2.0	1
1945	Kinetics and molecular mechanism of the Schonberg rearrangement. Computational and Theoretical Chemistry, 2022, 1208, 113585.	1.1	1
1946	Study of the alkyl-ï€ interaction between methane and few substituted pyrimidine systems using DFT, AIM and NBO calculations. Computational and Theoretical Chemistry, 2022, 1208, 113560.	1.1	6
1947	Measurement of Donor-Acceptor Interchange Tunnelling in Ar(H2O)2 using Rotational Spectroscopy and a Re-look at Its Structure and Bonding. Journal of Molecular Structure, 2022, 1252, 132094.	1.8	1
1948	DFT study of 2D graphitic carbon nitride based preferential targeted delivery of levosimendan, a cardiovascular drug. Computational and Theoretical Chemistry, 2022, 1209, 113584.	1.1	6

#	Article	IF	CITATIONS
1949	Spodium bonds and metal–halogen···halogen–metal interactions in propagation of monomeric units to dimeric or polymeric architectures. Journal of Molecular Structure, 2022, 1252, 132144.	1.8	8
1950	Turning ON/OFF the fluorescence of the ESIPT state by changing the hydrogen bond distance and orientation in quinoline–pyrazole derivatives. Journal of Molecular Structure, 2022, 1252, 132146.	1.8	9
1951	Intermolecular (Isocyano group)···PtII interactions involving coordinated isocyanides in cyclometalated PtII complexes. Journal of Molecular Structure, 2022, 1253, 132230.	1.8	9
1952	Solvothermal synthesis and crystal structures of two Holmium(III)-5-Hydroxyisophthalate entangled coordination polymers and theoretical studies on the importance of π•••π stacking interactions. Journal of Molecular Structure, 2022, 1254, 132329.	1.8	10
1953	Adsorption of Sorbitan Ester Surfactant on Copper and Copper Oxidized Surfaces: A Density Functional Theory Study. SSRN Electronic Journal, 0, , .	0.4	0
1954	Origin of Ligand Effects on Stereoinversion in Pd-Catalyzed Synthesis of Tetrasubstituted Olefins. Journal of Organic Chemistry, 2021, 86, 18128-18138.	1.7	11
1955	Multicomponent Solids of DL-2-Hydroxy-2-phenylacetic Acid and Pyridinecarboxamides. Crystals, 2022, 12, 142.	1.0	4
1956	Structural design and physicochemical specifications exploring of the new di-cationic ionic liquids (D-ILs) composed of para-xylyl linked N-Methylimidazolium cation and various anions: a full M06–2X computational study. Theoretical Chemistry Accounts, 2022, 141, 1.	0.5	10
1957	Investigation of the adsorption properties of gemcitabine anticancer drug with metal-doped boron nitride fullerenes as a drug-delivery carrier: a DFT study. RSC Advances, 2022, 12, 2873-2887.	1.7	31
1958	Porphyrinâ€Based COF 2D Materials: Variable Modification of Sensing Performances by Postâ€Metallization. Angewandte Chemie, 0, , .	1.6	13
1959	Unveiling the synthesis of spirocyclic, tricyclic, and bicyclic triazolooxazines from intramolecular [3 + 2] azide-alkyne cycloadditions with a molecular electron density theory perspective. Structural Chemistry, 2022, 33, 555-570.	1.0	6
1960	Large interaction energy for the homodimer and the heterodimer extracted from the supramolecular chain of a bent trinuclear zinc( <scp>ii</scp> ) complex with a reduced Schiff base ligand. New Journal of Chemistry, 2022, 46, 1845-1856.	1.4	2
1961	A molecular electron density theory study of the higher-order cycloaddition reactions of tropone with electron-rich ethylenes. The role of the Lewis acid catalyst in the mechanism and pseudocyclic selectivity. New Journal of Chemistry, 2021, 46, 294-308.	1.4	4
1962	Dramatic differences in the conformational equilibria of chalcogen-bridged compounds: the case of diallyl ether <i>versus</i> diallyl sulfide. Physical Chemistry Chemical Physics, 2021, 24, 240-248.	1.3	3
1963	A radical approach to radicals. Acta Crystallographica Section D: Structural Biology, 2022, 78, 43-51.	1.1	0
1964	Importance of water and intramolecular interaction governs substantial blue shift of Csp2–H stretching frequency in complexes between chalcogenoaldehydes and water. RSC Advances, 2022, 12, 1998-2008.	1.7	2
1965	Recent advances on the tetrel bonding interaction in the solid state structure of lead complexes with hydrazine based bis-pyridine Schiff base ligands. Polyhedron, 2022, 216, 115670.	1.0	11
1966	Evaluation of the mechanism, regio-, and diastereoselectivity of aza-Diels–Alder reactions of 2H-azirine under a Lewis acid catalyst. Structural Chemistry, 2022, 33, 445	1.0	0

#	Article	IF	CITATIONS
1967	Dienylation of <i>N</i> -benzoylhydrazones with CF <sub>3</sub> -substituted homoallenylboronates in water. Organic and Biomolecular Chemistry, 2022, 20, 1386-1390.	1.5	0
1968	Heteroleptic Pd(II) and Pt(II) Complexes with Redox-Active Ligands: Synthesis, Structure, and Multimodal Anticancer Mechanism. Inorganic Chemistry, 2022, 61, 2105-2118.	1.9	26
1969	The mechanism and origin of selectivities for NHC-catalyzed synthesis of axially chiral benzothiophene/benzofuran-fused biaryls. Organic and Biomolecular Chemistry, 2022, 20, 1662-1670.	1.5	11
1970	A computational study of competing conformational selection and induced fit in an abiotic system. Physical Chemistry Chemical Physics, 2021, 24, 507-511.	1.3	1
1971	Interactions between typical functional groups of soil organic matter and mica (001) surface: A DFT study. Applied Clay Science, 2022, 216, 106374.	2.6	2
1972	Asymmetric synthesis of N–N axially chiral compounds <i>via</i> organocatalytic atroposelective <i>N</i> -acylation. Chemical Science, 2021, 13, 141-148.	3.7	53
1973	Experimental and computational evidence for stabilising parallel, offset Ï€[C(î€O)N(H)N]â< Ï€(phenyl) interactions in acetohydrazide derivatives. CrystEngComm, 2022, 24, 962-974.	1.3	0
1974	The Effect of Single-Atom Substitution on Structure and Band Gap in Organic Semiconductors. Crystal Growth and Design, 2022, 22, 1237-1243.	1.4	5
1975	Oxalic Acid, a Versatile Coformer for Multicomponent Forms with 9-Ethyladenine. Crystals, 2022, 12, 89.	1.0	3
1976	Halogen Bonding in Haspin-Halogenated Tubercidin Complexes: Molecular Dynamics and Quantum Chemical Calculations. Molecules, 2022, 27, 706.	1.7	2
1977	The effects of solvent nature and steric hindrance on the reactivity, mechanism and selectivity of the cationic iminoâ€Diels–Alder cycloaddition reaction between cationic 2â€azadienes and arylpropene. Journal of Physical Organic Chemistry, 0, , .	0.9	4
1978	Steric Hindrance Favors σ Dimerization over π Dimerization for Julolidine Dicyanomethyl Radicals. Journal of Organic Chemistry, 2022, 87, 1507-1511.	1.7	8
1979	Bifunctional Iminophosphorane-Catalyzed Enantioselective Sulfa-Michael Addition to Unactivated α,β-Unsaturated Amides. Journal of the American Chemical Society, 2022, 144, 1006-1015.	6.6	24
1980	Porphyrinâ€Based COF 2D Materials: Variable Modification of Sensing Performances by Postâ€Metallization. Angewandte Chemie - International Edition, 2022, 61, .	7.2	63
1981	Computer simulation applied to structural analysis and experimental applications of natural deep eutectic solvents. , 2022, , 281-297.		1
1982	Boosting Gold(I) Catalysis via Weak Interactions: New Fine-Tunable Impy Ligands. ACS Organic & Inorganic Au, 2022, 2, 229-235.	1.9	6
1983	Exploring the effect of nitrile substituent position on fluorescence quantum yield of ESIPT-based oxazoline derivatives: A TDDFT investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 272, 120953.	2.0	15
1984	Molecular insights into chirality transfer from double axially chiral phosphoric acid in a synergistic enantioselective intramolecular amination. Chemical Science, 2022, 13, 1323-1334.	3.7	6

#	Article	IF	CITATIONS
1985	How neocarcerand Octacid4 self-assembles with guests into irreversible noncovalent complexes and what accelerates the assembly. Communications Chemistry, 2022, 5, .	2.0	0
1986	A Theoretical Evaluation of the Behavior of Nitrosoamidine upon Reacting with Methoxy Butadiene, as Potential Heterodiene or Heterodienophile. Letters in Organic Chemistry, 2022, 19, .	0.2	0
1987	Syntheses, crystal structures and supramolecular assemblies of two Cu( <scp>ii</scp> ) complexes based on a new heterocyclic ligand: insights into C–H⋯Cl and π⋯΀ interactions. CrystEngComm, 2022, 24, 1598-1611.	1.3	17
1988	Enantioselective Pdâ€catalyzed allylic substitution using phosphiteâ€oxazoline PHOXâ€based ligands containing a methylene linker. European Journal of Inorganic Chemistry, 0, , .	1.0	2
1989	Chalcogen···Chalcogen Bonding in Molybdenum Disulfide, Molybdenum Diselenide and Molybdenum Ditelluride Dimers as Prototypes for a Basic Understanding of the Local Interfacial Chemical Bonding Environment in 2D Layered Transition Metal Dichalcogenides. Inorganics, 2022, 10, 11.	1.2	8
1990	Chiral <i>N</i> -triflylphosphoramide-catalyzed asymmetric hydroamination of unactivated alkenes: a hetero-ene reaction mechanism. Organic Chemistry Frontiers, 2022, 9, 1649-1661.	2.3	4
1991	Unraveling the mechanism and substituent effects on the N-heterocyclic carbene-catalyzed transformation reaction of enals and imines. Molecular Catalysis, 2022, 519, 112122.	1.0	8
1992	Spodium and tetrel bonds involving Zn(II)/Cd(II) and their interplay. Chemical Physics, 2022, 556, 111470.	0.9	6
1993	Theoretical investigation on the cycloaddition catalyzed by rhodium silylenoid to construct silicon-containing rings. Molecular Catalysis, 2022, 519, 112138.	1.0	1
1994	Independent gradient model based on Hirshfeld partition: A new method for visual study of interactions in chemical systems. Journal of Computational Chemistry, 2022, 43, 539-555.	1.5	794
1995	Steric paths in confined hydrogen molecule inside carbon nanorings and fullerenes. Computational and Theoretical Chemistry, 2022, 1209, 113590.	1.1	0
1996	Water binding to the atmospheric oxidation product methyl vinyl ketone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 270, 120846.	2.0	2
1997	Synthesis and characterization of Zinc(II) complex with ONO donor type new phenylpropanehydrazide based ligand: Crystal structure, Hirshfeld surface analysis, DFT, energy frameworks and molecular docking. Journal of Molecular Structure, 2022, 1255, 132429.	1.8	5
1998	Superalkali (Li2F, Li3F) doped Al12N12 electrides with enhanced static, dynamic nonlinear optical responses and refractive indices. Materials Science in Semiconductor Processing, 2022, 143, 106518.	1.9	23
1999	Computational discoveries of reaction mechanisms: recent highlights and emerging challenges. Organic and Biomolecular Chemistry, 2022, 20, 2028-2042.	1.5	4
2000	Exploring Supramolecular Assembly Space of Cationic 1,2,4-Selenodiazoles: Effect of the Substituent at the Carbon Atom and Anions. Molecules, 2022, 27, 1029.	1.7	15
2001	Weak intermolecular interactions of cysteine on BNNT, BNAINT and BC2NNT: a DFT investigation. Bulletin of Materials Science, 2022, 45, 1.	0.8	29
2002	Phosphorescent Complexes of {Mo <sub>6</sub> I <sub>8</sub> } <sup>4+</sup> and {W <sub>6</sub> I <sub>8</sub> } <sup>4+</sup> with Perfluorinated Aryl Thiolates featuring Unusual Molecular Structures. European Journal of Inorganic Chemistry, 2022, 2022, .	1.0	7

#	Article	IF	CITATIONS
2003	Alkynyl Sulfonium Salts Can Be Employed as Chalcogenâ€Bonding Catalysts and Generate Alkynyl Radicals under Blue‣ight Irradiation. Angewandte Chemie - International Edition, 2022, 61, .	7.2	36
2004	π–π Stacking Interaction of Metal Phenoxyl Radical Complexes. Molecules, 2022, 27, 1135.	1.7	4
2005	New Cd(II) complex derived from (1-methylimidazol-2-yl) methanol: Synthesis, crystal structure, spectroscopic study, DFT and TD-DFT calculations, antimicrobial activity and free-radical scavenging capacity. Journal of Molecular Structure, 2022, 1257, 132583.	1.8	3
2006	Alkynyl Sulfonium Salts Can Be Employed as Chalcogenâ€Bonding Catalysts and Generate Alkynyl Radicals under Blue‣ight Irradiation. Angewandte Chemie, 2022, 134, .	1.6	8
2007	Theoretical and experimental investigation of a pyrazole derivative- solvation effects, reactivity analysis and MD simulations. Chemical Physics Letters, 2022, 793, 139469.	1.2	7
2008	Extended Î <sup>2</sup> -Strands Contribute to Reversible Amyloid Formation. ACS Nano, 2022, 16, 2154-2163.	7.3	14
2009	Quantum Chemical Studies of Lewis-Acid Catalyzed Organic Chemical Reactions. Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry, 2022, 80, 115-125.	0.0	0
2010	Subsistence of diverse interactions of some biologically important molecules in aqueous ionic liquid solutions at various temperatures by experimental and theoretical investigation. Journal of Molecular Structure, 2022, 1257, 132571.	1.8	11
2011	2-Pyridylselenenyl versus 2-Pyridyltellurenyl Halides: Symmetrical Chalcogen Bonding in the Solid State and Reactivity towards Nitriles. Symmetry, 2021, 13, 2350.	1.1	14
2012	Intramolecular hydrogen transfer in DNA induced by site-selective resonant core excitation. Physical Chemistry Chemical Physics, 2022, 24, 7815-7825.	1.3	2
2013	Enhancing chalcogen bonding by metal coordination. Dalton Transactions, 2022, , .	1.6	9
2014	Unveiling the intramolecular [3 + 2] cycloaddition reactions of <i>C</i> , <i>N</i> -disubstituted nitrones from the molecular electron density theory perspective. New Journal of Chemistry, 2022, 46, 7721-7733.	1.4	9
2015	Experimental and theoretical insights into the formation of weak hydrogen bonds and H⋯H bonding interactions in the solid-state structure of two eucalyptol derivatives. New Journal of Chemistry, 2022, 46, 5690-5704.	1.4	3
2016	Design of selective divalent chain transfer agents for coordinative chain transfer polymerization of ethylene and its copolymerization with butadiene. Polymer Chemistry, 2022, 13, 1970-1977.	1.9	11
2017	Insight into the Cation-Regulated MechanismÂFor the Hydration of Propargyl Alcohols Catalyzed by [Bu4p+][Im-]. SSRN Electronic Journal, 0, , .	0.4	0
2018	The influence of <scp>l</scp> -aspartic acid on calcium carbonate nucleation and growth revealed by <i>in situ</i> liquid phase TEM. CrystEngComm, 2022, 24, 2602-2614.	1.3	8
2019	Metallophilic interactions in silver( <scp>i</scp> ) dicyanoaurate complexes. Dalton Transactions, 2022, , .	1.6	1
2020	Do 2-coordinate iodine( <scp>i</scp> ) and silver( <scp>i</scp> ) complexes form nucleophilic iodonium interactions (NIIs) in solution?. Chemical Communications, 2022, 58, 4977-4980.	2.2	9

#	Article	IF	CITATIONS
2021	Insight into the New Catalytic Species for the Hydration of Propargyl Alcohols Catalyzed by [Bu4p+][Im-]. SSRN Electronic Journal, 0, , .	0.4	0
2022	Torsional chirality and molecular recognition: the homo and heterochiral dimers of thenyl and furfuryl alcohol. Physical Chemistry Chemical Physics, 2022, 24, 8999-9006.	1.3	4
2023	Cycloaddition of isoselenocyanates to sodium and magnesium metallacycles. Dalton Transactions, 2022, 51, 4113-4121.	1.6	10
2024	Structural topologies involving energetically significant antiparallel Ï€-stacking and unconventional N(nitrile)â<Ï€(fumarate) contacts in dinuclear Zn( <scp>ii</scp> ) and polymeric Mn( <scp>ii</scp> ) compounds: antiproliferative evaluation and theoretical studies. New Journal of Chemistry, 2022, 46, 5296-5311.	1.4	7
2025	Synthesis, spectroscopic findings and crystal engineering of Pb( <scp>ii</scp> )–Salen coordination polymers, and supramolecular architectures engineered by σ-hole/spodium/tetrel bonds: a combined experimental and theoretical investigation. RSC Advances, 2022, 12, 6352-6363.	1.7	25
2026	Combined crystallographic and computational investigation of the solvent disorder present in a new tipiracil hydrochloride methanol solvate–hydrate. CrystEngComm, 0, , .	1.3	1
2027	Mechanistic exploration of CO <sub>2</sub> conversion to dimethoxymethane (DMM) using transition metal (Co, Ru) catalysts: an energy span model. Physical Chemistry Chemical Physics, 2022, 24, 8387-8397.	1.3	9
2028	lodine( <scp>i</scp> ) complexes incorporating sterically bulky 2-substituted pyridines. RSC Advances, 2022, 12, 8674-8682.	1.7	6
2029	Static discrete disorder in the crystal structure of iododiflunisal: on the importance of hydrogen bond, halogen bond and π-stacking interactions. CrystEngComm, 0, , .	1.3	3
2030	Solvent-driven structural topologies in phenanthroline-based co-crystals of 2n( <scp>ii</scp> ) involving fascinating infinite chair-like {[(bzH) <sub>4</sub> Cl <sub>2</sub> ] <sup>2â<sup>°</sup></sup> } <sub><i>n</i></sub> assemblies and unconventional layered infinite {bz-H <sub>2</sub> O-Cl} <sub><i>n</i></sub> anion-water clusters:	1.4	4
2031	Computational Chemistry as a Conceptual Game Changer: Understanding the Role of London Dispersion in Hexaphenylethane Derivatives (Gomberg Systems). Israel Journal of Chemistry, 2022, 62, .	1.0	12
2032	Strength and Nature of Hostâ€Guest Interactions in Metalâ€Organic Frameworks from a Quantumâ€Chemical Perspective. ChemPhysChem, 2022, 23, .	1.0	8
2033	Analysis of Weak Interactions in Crystals of Fenamic Acids–Ethacridine Complexes. Crystal Growth and Design, 2022, 22, 1554-1570.	1.4	0
2034	Planar Chiral 1,3-Disubstituted Ferrocenyl Phosphine Gold(I) Catalysts. ACS Catalysis, 2022, 12, 3317-3322.	5.5	17
2035	Theoretical Insights into Nitrogen-Doped Graphene-Supported Fe, Co, and Ni as Single-Atom Catalysts for CO <sub>2</sub> Reduction Reaction. Journal of Physical Chemistry C, 2022, 126, 4338-4346.	1.5	24
2036	Mo(VI) Potential Metallodrugs: Explaining the Transport and Cytotoxicity by Chemical Transformations. Inorganic Chemistry, 2022, 61, 4513-4532.	1.9	12
2037	Insights on structure and interactions of 2-amino-4-methoxy-6-methylpyrimidinium salts with 4-aminosalicylate and 5-chlorosalicylate: a combined experimental and theoretical charge–density analysis. Acta Crystallographica Section C, Structural Chemistry, 2022, 78, 181-191.	0.2	3
2038	Quantum Mechanical Investigation into the Adsorption Pattern of Clomipramine and Methotrimeprazine HCl with Graphene and Fullerene. Polycyclic Aromatic Compounds, 2023, 43, 2219-2232.	1.4	7

#	Article	IF	CITATIONS
2039	Integrated Experimental and Computational Studies on the Organocatalytic Kinetic Resolution of β-Unfunctionalized Primary Alcohols Using a Chiral 1,2-Diamine: The Importance of Noncovalent Interactions. Journal of Organic Chemistry, 2022, 87, 4468-4475.	1.7	2
2040	Exploiting the Redox Activity of MIL-100(Fe) Carrier Enables Prolonged Carvacrol Antimicrobial Activity. ACS Applied Materials & Interfaces, 2022, 14, 10758-10768.	4.0	11
2041	Hydrogen-Bond-Assisted Diels–Alder Kinetics or Self-Healing in Reversible Polymer Networks? A Combined Experimental and Theoretical Study. Molecules, 2022, 27, 1961.	1.7	5
2042	Giant Supramolecular Synthons via Cyclic Halogen··À·Halogen Contacts in Substituted <i>o</i> -Xylenes. Crystal Growth and Design, 2022, 22, 2318-2327.	1.4	5
2043	Analysis of Conformational Preferences in Caffeine. Molecules, 2022, 27, 1937.	1.7	1
2044	Synthesis and Theoretical Study of New Guanylated Cyclophosphazenes and Their Use in the CO2 Fixation into Styrene Carbonate. Journal of Inorganic and Organometallic Polymers and Materials, 2022, 32, 1724-1735.	1.9	1
2045	Inclusion of thymol into cucurbiturils: density functional theory approach with dispersion correction and natural bond orbital analysis. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 0, , 1.	0.9	3
2046	Efficient Synthesis for a Wide Variety of Patellamide Derivatives and Phosphatase Activity of Copperâ€Patellamide Complexes. Chemistry - A European Journal, 2022, 28, .	1.7	6
2047	Carbon-Centered Hydrogen Bonds in Proteins. Journal of Chemical Information and Modeling, 2022, 62, 1998-2008.	2.5	17
2048	Interaction of Anagrelide drug molecule on pristine and doped boron nitride nanocages: a DFT, RDG, PCM and QTAIM investigation. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3413-3429.	2.0	8
2049	Gauging the Steric Effects of Silyl Groups with a Molecular Balance. Journal of Organic Chemistry, 2022, 87, 4670-4679.	1.7	14
2050	Effect of hydrogen bonds and CF3 group on the regioselectivity and mechanism of [3 + 2] cycloaddition reactions between nitrile oxide and 2,4-disubstitutedÂcyclopentenes. A MEDT study. Journal of Molecular Modeling, 2022, 28, 104.	0.8	4
2051	Synthesis Characterization and X-ray Structure of 2-(2,6-Dichlorophenylamino)-2-imidazoline Tetraphenylborate: Computational Study. Applied Sciences (Switzerland), 2022, 12, 3568.	1.3	8
2052	Rotational Spectroscopy of 2â€Furoic Acid and Its Dimer: Conformational Distribution and Double Proton Tunneling. ChemPhysChem, 2022, , .	1.0	1
2053	Azide–Alkyne Interactions: A Crucial Attractive Force for Their Preorganization for Topochemical Cycloaddition Reaction. Chemistry - A European Journal, 2022, 28, .	1.7	11
2054	The study of Letrozole adsorption upon CCT nanotube: A DFT/TD-DFT and spectroscopic (excited states) Tj ETQq1	1.0.7843	14 rgBT /0
2055	Toward Density-Based and Simultaneous Description of Chemical Bonding and Noncovalent Interactions with Pauli Energy. Journal of Physical Chemistry A, 2022, 126, 2437-2444.	1.1	14
2056	Selective semi-hydrogenation of internal alkynes catalyzed by Pd–CaCO3 clusters. Journal of Catalysis, 2022, 408, 43-55.	3.1	29

#	Article	IF	CITATIONS
2057	Sensing behaviour of monocyclic C18 and B9N9 analogues toward chemical warfare agents (CWAs); quantum chemical approach. Surfaces and Interfaces, 2022, 30, 101912.	1.5	13
2058	Potential sensing of toxic chemical warfare agents (CWAs) by twisted nanographenes: A first principle approach. Science of the Total Environment, 2022, 824, 153858.	3.9	41
2059	Interaction of Fluorouracil drug with boron nitride nanotube, Al doped boron nitride nanotube and BC2N nanotube. Computational and Theoretical Chemistry, 2022, 1212, 113699.	1.1	22
2060	Exploring the potential energy surface of nCO2 (nÂ=Â1–5) capture by imidazole-and fluorine-based ionic liquids: A DFT study. Journal of Molecular Liquids, 2022, 356, 119022.	2.3	1
2061	Pyrolysis mechanism law of β-O-4 lignin dimer model compounds: A density functional theory study. Industrial Crops and Products, 2022, 180, 114746.	2.5	10
2062	Schistosomicidal evaluation of synthesized bromo and nitro chalcone derivatives. Journal of Molecular Structure, 2022, 1258, 132647.	1.8	2
2063	Microwave-enhanced synthesis of 26-amino-22-oxocholestanes and their cytotoxic activity. Steroids, 2022, 183, 109030.	0.8	3
2064	Spectroscopic analyses on an azatricycloderivative by DFT with different solvents, reactivity analysis and MD simulations. Journal of Molecular Structure, 2022, 1260, 132845.	1.8	0
2065	Adsorption of sorbitan ester surfactant on copper and Cuprous oxide surfaces: A density functional theory study. Applied Surface Science, 2022, 589, 153061.	3.1	2
2066	Hydrogen vs. halogen bonding in crystals of 2,5-dibromothiophene-3-carboxylic acid derivatives. Journal of Molecular Structure, 2022, 1260, 132785.	1.8	2
2067	Nanocellulose bio-based composites for the removal of methylene blue from water: An experimental and theoretical exploration. Journal of Molecular Liquids, 2022, 357, 119089.	2.3	6
2068	Spectroscopic and theoretical studies of some 2-(2′-ethylsulfanyl)acetyl-5-substituted furans and thiophenes. Journal of Molecular Structure, 2022, 1261, 132895. Dynamical and mechanical stability, electronic properties, bonding and weak interactions analysis of	1.8	1
2069	new compounds MgS2 and MgSe2 in <mml:math <br="" xmlns:mml="http://www.w3.org/1998/Math/MathML">altimg="si1.svg"&gt;<mml:mrow><mml:mtext>Pa</mml:mtext><mml:mover accent="true"&gt;<mml:mn>3</mml:mn><mml:mo stretchy="true"&gt;â€34</mml:mo </mml:mover </mml:mrow></mml:math> space group structure: Ab initio	1.9	12
2070	study. Materials Science in Semiconductor Processing, 2022, 146, 106659. <b>N-Heterocyclic Carbene-Photocatalyzed Tricomponent Regioselective 1,2-Diacylation of Alkenes Illuminates the Mechanistic Details of the Electron Donor–Acceptor Complex-Mediated Radical Relay Processes</b> . ACS Catalysis, 2022, 12, 285-294.	5.5	41
2072	Perfluorination of Aromatic Compounds Reinforce Their van der Waals Interactions with Rare Gases: The Rotational Spectrum of Pentafluoropyridine-Ne. Molecules, 2022, 27, 17.	1.7	3
2073	Allene C(sp <sup>2</sup> )–H Activation and Alkenylation Catalyzed by Palladium. Journal of the American Chemical Society, 2021, 143, 21705-21712.	6.6	25
2074	Mechanism and Design Principles for Controlling Stereoselectivity in the Copolymerization of CO <sub>2</sub> /Cyclohexene Oxide by Indium(III) Phosphasalen Catalysts. ACS Catalysis, 2021, 11, 15244-15251.	5.5	7
2075	Novel Polymorphic Cocrystals of the Non-Steroidal Anti-Inflammatory Drug Niflumic Acid: Expanding the Pharmaceutical Landscape. Pharmaceutics, 2021, 13, 2140.	2.0	9

	Ci	CITATION REPORT		
#	Article	IF		CITATIONS
2076	On the Quantum Chemical Nature of Lead(II) "Lone Pair― Molecules, 2022, 27, 27.	1.7	,	1
2077	Polymorphism in the 1/1 Pterostilbene/Picolinic Acid Cocrystal. Crystal Growth and Design, 2022, 22, 590-597.	1.4	}	10
2078	Inorganic–organic {d <sub><i>z</i><sup>2</sup></sub> -M <sup>II</sup> S <sub>4</sub> }â<¯i€-hole in reverse sandwich structures: the case of cocrystals of group 10 metal dithiocarbamates with electron-deficient arenes. Inorganic Chemistry Frontiers, 2022, 9, 2869-2879.	e stacking 3.0	)	9
2079	A DFT study of NHC-catalyzed reactions between 2-bromo-2-enals and acylhydrazones: mechanisms, a chemo- and stereoselectivities. New Journal of Chemistry, 2022, 46, 9146-9154.	and 1.4	ł	3
2080	Identification of natural flavonoids as novel EGFR inhibitors using DFT, molecular docking, and molecular dynamics. New Journal of Chemistry, 2022, 46, 9735-9744.	1.4	ŀ	13
2081	Hydrogen Atom Transfer Driven Enantioselective Minisci Reaction of Alcohols. Angewandte Chemie - International Edition, 2022, 61, .	7.2		29
2082	Proâ€Pro Dipeptideâ€Thiourea Organocatalyst in the Mannich Reaction between αâ€Imino Esters and Pyruvates. European Journal of Organic Chemistry, 2022, 2022, .	1 1.2	2	2
2083	Impact of Remdesivir Incorporation along the Primer Strand on SARS-CoV-2 RNA-Dependent RNA Polymerase. Journal of Chemical Information and Modeling, 2022, 62, 2456-2465.	2.5	5	7
2084	Experimental and Computational Structural Studies of 2,3,5-Trisubstituted and 1,2,3,5-Tetrasubstitute Indoles as Non-Competitive Antagonists of GluK1/GluK2 Receptors. Molecules, 2022, 27, 2479.	ed 1.7	,	3
2086	Hydrogen Atom Transfer Driven Enantioselective Minisci Reaction of Alcohols. Angewandte Chemie, 0	' 1.6	5	1
2087	Assessment of alkali and alkaline earth metals doped cubanes as high-performance nonlinear optical materials by first-principles study. Journal of Science: Advanced Materials and Devices, 2022, 7, 10045	57. <sup>1.5</sup>	5	8
2088	A Copper(II)â€Nitrite Complex Hydrogenâ€Bonded to a Protonated Amine in the Secondâ€Coordinationâ€Sphere. European Journal of Inorganic Chemistry, 2022, 2022, .	1.0	)	3
2089	Supramolecular aggregation of lead(II) perchlorate and a thiosemicarbazide derivative linked by a myriad of non-covalent interactions. Inorganica Chimica Acta, 2022, 538, 120974.	1.2	2	4
2090	Reaction mechanism of the gas-phase pyrolysis of N – Acetylthiourea and N, N'–diacetylthiou theoretical study based in density functional theory. Computational and Theoretical Chemistry, 2022, 1212, 113702.	rea: A 1.1		0
2091	Jet-cooled laser spectroscopy and solid-state vibrational circular dichroism of the cyclo-(Tyr-Phe) diketopiperazine dipeptide. Journal of Molecular Structure, 2022, 1262, 133059.	1.8	3	8
2092	Are metal dopant and ligands efficient to optimize the adsorption rate of CH4, H2 and H2S on IRMOF Insights from factorial design. Computational Materials Science, 2022, 210, 111438.	s? 1.4		5
2096	Endo―and exohedral complexes of superphane with cations. Journal of Computational Chemistry, 20 43, 1120-1133.	)22, 1.5	5	3
2097	On the energetic stability of halogen bonds involving metals: implications in crystal engineering. CrystEngComm, 2022, 24, 4440-4446.	1.3	3	15

	Сп	CITATION REPORT	
#	Article	IF	CITATIONS
2098	Porous liquids $\hat{a} \in $ the future is looking emptier. Chemical Science, 2022, 13, 5042-5054.	3.7	22
2099	Computational insights on the origin of enantioselectivity in reactions with diarylprolinol silyl ether catalysts <i>via</i> a radical pathway. Organic Chemistry Frontiers, 2022, 9, 3730-3738.	2.3	2
2100	Computational insight into the mechanism and stereoselectivity of cycloaddition between donor–acceptor spirocyclopropane and aldehyde catalyzed by BrÃ,nsted acid TsOH. Organic and Biomolecular Chemistry, 2022, 20, 4006-4015.	1.5	3
2101	Insight into non-covalent interactions in a [Cu(N <sub>3</sub> ) <sub>4</sub> ] <sup>2â^'</sup> bridg hetero-pentanuclear copper( <scp>ii</scp> )/sodium complex with special emphasis on the strong CHâ<ï€[Cu(N <sub>3</sub> ) <sub>4</sub> ] interactions. New Journal of Chemistry, 2022, 46, 11286-	1.4	7
2102	Water-Dispersible Polymer Coated Silica Nanoparticle for Turn-On Fluorometric Detection of Cephalexin. SSRN Electronic Journal, 0, , .	0.4	0
2103	Mixed superalkalis are a better choice than pure superalkalis for B <sub>12</sub> N <sub>12</sub> nanocages to design high-performance nonlinear optical materials. Dalton Transactions, 2022, 51, 8437-8453.	1.6	10
2104	Insight into Spodium–π Bonding Characteristics of the MX2â<Ï€ (M = Zn, Cd and Hg; X = Cl, Br and Complexes—A Theoretical Study. Molecules, 2022, 27, 2885.	l) 1.7	4
2105	Quantum chemistry study in metallophilic interactions on complexes based in Au(I)-Pb(II) and Au(I)-Bi(III). Molecular Simulation, 0, , 1-11.	0.9	0
2106	Experimental/Computational Study on the Impact of Fluorine on the Structure and Noncovalent Interactions in the Monohydrated Cluster of <i>ortho</i> -Fluorinated 2-Phenylethylamine. Journal of the American Chemical Society, 2022, 144, 8337-8346.	6.6	4
2107	Aurophilic Interactions in Cationic Three-Coordinate Gold(I) Bipyridyl/Isocyanide Complex. Crystals, 2022, 12, 613.	1.0	7
2108	London Dispersion Favors Sterically Hindered Diarylthiourea Conformers in Solution. Angewandte Chemie, 0, , .	1.6	2
2109	Harnessing Greenhouse Gases Absorption by Doped Fullerenes with Externally Oriented Electric Field. Molecules, 2022, 27, 2968.	1.7	3
2110	A DFT investigation on theranostic potential of alkaline earth metal doped phosphorenes for ifosfamide anti-cancer drug. Applied Surface Science, 2022, 596, 153618.	3.1	14
2111	Solvent effects on the molecular structure of isolated lignins of Eucalyptus nitens wood and oxidative depolymerization to phenolic chemicals. Polymer Degradation and Stability, 2022, 201, 1099	973. <sup>2.7</sup>	3
2112	Molecular basis for the initiation of DNA primer synthesis. Nature, 2022, 605, 767-773.	13.7	11
2113	Interaction of the Serine Amino Acid with BNNT, BNAINT, and BC2NNT. Arabian Journal for Science and Engineering, 0, , .	1.7	1
2114	Removal of Methyl Violet Dye by Adsorption Process on Hydrogen Titanate Nanotubes: Experimental-Theoretical Study. Water, Air, and Soil Pollution, 2022, 233, .	1.1	1
2115	The role of weak intermolecular interactions in photophysical behavior of isocoumarins on the example of their interaction with cyclic trinuclear silver(I) pyrazolate. Inorganica Chimica Acta, 2022, 539, 121004.	1.2	4

#	Article	IF	CITATIONS
2116	London Dispersion Favors Sterically Hindered Diarylthiourea Conformers in Solution. Angewandte Chemie - International Edition, 2022, 61, .	7.2	16
2117	External Electric Field Effect on the Strength of σ-Hole Interactions: A Theoretical Perspective in Likeâ< Like Carbon-Containing Complexes. Molecules, 2022, 27, 2963.	1.7	4
2118	Increasing Complexity in a Conformer Space Step-by-Step: Weighing London Dispersion against Cationâ^'l€ Interactions. Journal of the American Chemical Society, 2022, 144, 9007-9022.	6.6	13
2119	NHC Catalyzed β-Carbon functionalization of carboxylic esters towards formation of δ-Lactams: A mechanistic study. Molecular Catalysis, 2022, 524, 112311.	1.0	0
2120	A DFT approach towards therapeutic potential of phosphorene as a novel carrier for the delivery of felodipine (cardiovascular drug). Computational and Theoretical Chemistry, 2022, 1212, 113724.	1.1	7
2121	In vitro and in silico analysis of galanthine from Zephyranthes carinata as an inhibitor of acetylcholinesterase. Biomedicine and Pharmacotherapy, 2022, 150, 113016. Study of phase transitions and lattice dynamics, elastic and electronic properties, bonding and weak	2.5	7
2122	interactions analysis of YCuS2 in P212121, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"&gt; <mml:mrow> <mml:mtext> </mml:mtext> <mml:mover accent="true"&gt; <mml:mn> 4 </mml:mn> <mml:mo< td=""><td>1.9</td><td>3</td></mml:mo<></mml:mover </mml:mrow></mml:math 	1.9	3
2123	stretchy="true">‾ <mml:mn>2</mml:mn> <mml:mtext>d</mml:mtext> α-(1,2,3-Triazolyl)-acetophenone: Synthesis and theoretical studies of crystal and 2,4-dinitrophenylhydrazine cocrystal structures. Journal of Molecular Structure, 2022, 1264, 133225.	> 1.8	ath>and <mr 4</mr 
2124	Estimation of the ability of the π-system of pseudohalides (azide and thiocyanate) to participate in CH··Ĩ€ interactions in cyclic hetero-tetranuclear cobalt(III)/sodium and linear trinuclear mixed valence cobalt(III/II/III) complexes. Polyhedron, 2022, 222, 115862.	1.0	4
2125	Noncovalent interactions in proteins and nucleic acids: beyond hydrogen bonding and π-stacking. Chemical Society Reviews, 2022, 51, 4261-4286.	18.7	57
2126	Lanthanide coordination polymers functionalized by 5-nitroisophthalic acid: Synthesis, structure-DFT correlation and photoluminescent sensor of Cd2+ ion. Journal of Solid State Chemistry, 2022, 312, 123229.	1.4	5
2127	Kinetics and Mechanism of the Barton-Kellogg Oleï¬nation: A Computational DFT Study Using CTST Theory and Topological Approaches. New Journal of Chemistry, 0, , .	1.4	0
2128	Halogen-Bonded Cocrystals of 1,3,5-Triiodo-2,4,6-trifluorobenzene and Structural Isomers of Benzoylpyridine. Crystal Growth and Design, 2022, 22, 3981-3989.	1.4	6
2129	Asymmetric Coordination Mode of Phenanthroline-like Ligands in Gold(I) Complexes: A Case of the Antichelate Effect. Crystal Growth and Design, 2022, 22, 3882-3895.	1.4	3
2130	Diastereoselective Indole-Dearomative Cope Rearrangements by Compounding Minor Driving Forces. Organic Letters, 2022, 24, 3726-3730.	2.4	6
2131	Ratiometric pH Sensing, Photophysics, and Cell Imaging of Nonaromatic Light-Emitting Polymers. ACS Applied Bio Materials, 2022, 5, 2990-3005.	2.3	9
2132	Mechanism and Origin of Enantioselectivity in Bifunctional Squaramide atalyzed αâ€Thiolation of Azlactones. European Journal of Organic Chemistry, 0, , .	1.2	1
2133	Secondary Coordination Sphere Influences the Formation of Fe(III)-O or Fe(III)-OH in Nitrite Reduction: A Synthetic and Computational Study. Inorganic Chemistry, 2022, 61, 8182-8192.	1.9	8

#	Article	IF	CITATIONS
2134	The physical nature of the ultrashort spike–ring interaction in iron maiden molecules. Journal of Computational Chemistry, 2022, 43, 1206-1220.	1.5	6
2135	Theoretical investigation of the cooperative effect of solvent: a case study. Physical Chemistry Chemical Physics, 0, , .	1.3	4
2136	pH-induced structural variations of two new Mg(II)-PDA complexes: experimental and theoretical studies. Journal of Molecular Structure, 2022, 1265, 133373.	1.8	7
2137	Exploration of noncovalent interactions in the solid state structures of carboxylate bridged trinuclear mixed valence cobalt complexes using computational tools based on the topological analysis of the electron density. Polyhedron, 2022, 223, 115910.	1.0	5
2138	Installing a molecular truss beam stabilizes MOF structures. Npj Computational Materials, 2022, 8, .	3.5	3
2139	Exploration of supramolecular and theoretical aspects of two new Cu(II) complexes: On the importance of lone pair···π(chelate ring) and π···Ĩ€(chelate ring) interactions. Journal of Molecular Structure, 2022, 1265, 133358.	1.8	5
2140	Analysis of the host–guest complex formation involving bridged hexameric pyridinium–phenyl rings in the HexaCage6+ host in suit[3]ane: insights from dispersion-corrected DFT calculations for a nanometric mechanically interlocked device. Journal of Nanostructure in Chemistry, 0, , .	5.3	2
2141	Synthesis, crystal structure and noncovalent study of 1,5-Bis[1-(4-Fluorophenyl)ethylidene]-carbohidrazide. Journal of Molecular Structure, 2022, 1265, 133347.	1.8	1
2142	Importance of R-CH3⋯O tetrel bonding and vinyl⋯aryl stacking interactions in stabilizing the crystal packing of 2',4'-dihydroxy-3'-methoxychalcone: Exploration of antileishmanial activity and molecular docking studies. Journal of Molecular Structure, 2022, 1265, 133357.	1.8	1
2143	Highly selective acid-catalyzed olefin isomerization of limonene to terpinolene by kinetic suppression of overreactions in a confined space of porous metal–macrocycle frameworks. Chemical Science, 2022, 13, 8752-8758.	3.7	6
2144	The promoter role of sulfur in carbon nanotube growth. Dalton Transactions, 2022, 51, 9256-9264.	1.6	5
2145	Characterizing the n→ï€* interaction of pyridine with small ketones: a rotational study of pyridineâ⊂acetone and pyridineâ⊂2-butanone. Physical Chemistry Chemical Physics, 2022, 24, 15484-15493.	1.3	5
2146	Nickel and Palladium Complexes of a PP(O)P Pincer Ligand Based upon a <i>peri</i> -Substituted Acenaphthyl Scaffold and a Secondary Phosphine Oxide. Inorganic Chemistry, 2022, 61, 8406-8418.	1.9	3
2147	Sterically Hindered Tellurium(IV) Catecholate as a Lewis Acid. Inorganic Chemistry, 0, , .	1.9	6
2148	Comprehensive Study of the Chemistry behind the Stability of Carboxylic SWCNT Dispersions in the Development of a Transparent Electrode. Nanomaterials, 2022, 12, 1901.	1.9	3
2149	Enhanced steric effect and desolvation process on organic solvent nanofiltration: A mechanism study for removing anionic dyes. Chemical Engineering Journal, 2022, 446, 137360.	6.6	4
2150	Hydrogen Bonding with Polonium. Physical Chemistry Chemical Physics, 0, , .	1.3	6
2151	Janus faced fluorocyclohexanes for supramolecular assembly: synthesis and solid state structures of equatorial mono-, di- and tri alkylated cyclohexanes and with tri-axial C–F bonds to impart polarity. Chemical Communications, 2022, 58, 7968-7971.	2.2	6

#	Article	IF	CITATIONS
2152	Combined computational/experimental investigation of new cocrystals of the drug bosentan. CrystEngComm, 2022, 24, 5105-5111.	1.3	7
2153	Nhc-Catalyzed [3+4] Annulation between 2-Dromoenal and Aryl 1,2-Diamine: Insights into Mechanisms, Chemo and Stereoselectivities. SSRN Electronic Journal, 0, , .	0.4	0
2154	HYDROGEN BONDING IN THE CRYSTAL OF 1,1′-((1E,1′E)-(PYRIDINE-3,4-DIYLBIS) Tj ETQq0 0 0 rgBT /Overloo EXPERIMENTAL AND THEORETICAL STUDY. Journal of Structural Chemistry, 2022, 63, 626-633.	ck 10 Tf 50 0.3	) 667 Td ((A2 1
2155	Hydrophobic π-π stacking interactions and hydrogen bonds drive self-aggregation of luteolin in water. Journal of Molecular Graphics and Modelling, 2022, 116, 108243.	1.3	6
2156	Single Metal Atom Catalysts and ORR: H-Bonding, Solvation, and the Elusive Hydroperoxyl Intermediate. ACS Catalysis, 2022, 12, 7950-7959.	5.5	4
2157	Synthesis of a donor–acceptor heterodimer via trifunctional completive self-sorting. Nature Communications, 2022, 13, .	5.8	2
2158	Synthesis, structural and DFT studies on thiosemicarbazone-based dioxomolybdenum(VI) complexes with co-ligands. Journal of Coordination Chemistry, 0, , 1-19.	0.8	0
2159	Unveiling the <i>cbâ€type</i> Intramolecular [3+2] Cycloaddition Reactions of Fluorinated Azomethine Ylides to Ester Carbonyls with a Molecular Electron Density Theory Perspective. ChemistrySelect, 2022, 7, .	0.7	1
2160	A Molecular Electron Density Theory Study of the [3+2] Cycloaddition Reaction of Pseudo(mono)radical Azomethine Ylides with Phenyl Vinyl Sulphone. Organics, 2022, 3, 122-136.	0.6	10
2161	Enantioselective Cascade Michael/Hemiaminal Formation of α,β-Unsaturated Iminoindoles with Aldehydes Using a Chiral Aminomethylpyrrolidine Catalyst Bearing a SO <sub>2</sub> C <sub>6</sub> F <sub>5</sub> Group as a Strongly Electron Withdrawing ArvIsulfonyl Group, ACS Catalysis, 2022, 12, 7436-7442.	5.5	8
2162	Revision of the Crystal Structure of the Orthorhombic Polymorph of Oxyma: On the Importance of ï€â€"Hole Interactions and Their Interplay with H–Bonds. Crystals, 2022, 12, 823.	1.0	1
2163	Through-Bond-Driven Through-Space Interactions in a Fullerene C <sub>60</sub> Noncovalent Dyad: An Unusual Strong Binding between Spherical and Planar π Electron Clouds and Culmination of Dyadic Fractals. Journal of Physical Chemistry A, 2022, 126, 3629-3641.	1.1	4
2164	Synthesis of Platinum-Containing Conjugated Polymers Bearing Chiral Phosphine Ligands. Study of Geometries and Intermolecular Interactions Leading to Aggregation. Organometallics, 2022, 41, 1699-1709.	1.1	7
2165	Lanthanum doped corannulenes with enhanced static and dynamic nonlinear optical properties: A first principle study. Physica B: Condensed Matter, 2022, 641, 414088.	1.3	8
2166	<i>N</i> -Methylation of Aniline Derivatives with CO <sub>2</sub> and Phenylsilane Catalyzed by Lanthanum Hydridotriarylborate Complexes bearing a Nitrogen Tridentate Ligand. ACS Catalysis, 2022, 12, 8220-8228.	5.5	6
2168	Conformationally Fixed Chiral Bisphosphine Ligands by Steric Modulators on the Ligand Backbone: Selective Synthesis of Strained 1,2-Disubstituted Chiral <i>cis</i> -Cyclopropanes. Journal of the American Chemical Society, 2022, 144, 10483-10494.	6.6	20
2169	Insights into solvation effects, spectroscopic, Hirshfeld surface Analysis, reactivity analysis and anti-Covid-19 ability of doxylamine succinate: Experimental, DFT, MD and docking simulations. Journal of Molecular Liquids, 2022, 361, 119609.	2.3	11
2170	Terephthalato and succinato bridged Mn(II) and Zn(II) coordination polymers involving structure-guiding H-bonded tetrameric assemblies: Antiproliferative evaluation and theoretical studies. Polyhedron, 2022, 224, 115982.	1.0	3

#	Article	IF	CITATIONS
2171	Structural characterization and computational investigations of three fluorine-containing ligands with a terphenyl core. Journal of Molecular Structure, 2022, 1266, 133474.	1.8	0
2172	An induced-fit model for asymmetric organocatalytic reactions: a case study of the activation of olefins <i>via</i> chiral BrĂ,nsted acid catalysts. Chemical Science, 2022, 13, 8848-8859.	3.7	8
2173	Nature and Role of Formal Charge of the Ion Inclusion in Hexanuclear Platinium(Ii) Host-Guest Species. Insights from Relativistic Dft Calculations. SSRN Electronic Journal, 0, , .	0.4	0
2174	Adsorption of Glyphosate on Graphene and Functionalized Graphenes: A Dft Study. SSRN Electronic Journal, 0, , .	0.4	0
2175	Understanding the n → π* non-covalent interaction using different experimental and theoretical approaches. Physical Chemistry Chemical Physics, 0, , .	1.3	6
2176	Centroidâ<̄centroid and hydrogen bond interactions as robust supramolecular units for crystal engineering: X-ray crystallographic, computational and urease inhibitory investigations of 1,2,4-triazolo[3,4-a]phthalazines. CrystEngComm, 0, , .	1.3	5
2177	Shape and topology optimization for maximum probability domains in quantum chemistry. Numerische Mathematik, 2022, 151, 1017-1064.	0.9	0
2178	Solvent-Mediated Charge Transfer Dynamics of a Model Brown Carbon Aerosol Chromophore: Photophysics of 1-Phenylpyrrole Induced by Water Solvation. Journal of Physical Chemistry A, 2022, 126, 4313-4325.	1.1	2
2179	Elaborating the mechanism of a highly selective fluorescent â€~turn-on' probe to detect the group IIIA ions: a detailed time-dependent density functional theory study. Theoretical Chemistry Accounts, 2022, 141, .	0.5	0
2180	Antiparallel π··Â-Ï€ and Câ^'H···Hâ^'C contacts in a novel Zn(II) coordination solid involving Ï€-hole tetrel bonding interactions: A combined experimental and theoretical study, Hirshfeld surface analysis, molecular docking and potential drug property. Journal of Molecular Structure, 2022, 1268, 133686.	1.8	4
2181	Nickel atalyzed Enantioselective Reductive Alkyl arbamoylation of Internal Alkenes. Angewandte Chemie, 0, , .	1.6	0
2182	Nickel atalyzed Enantioselective Reductive Alkyl arbamoylation of Internal Alkenes. Angewandte Chemie - International Edition, 2022, 61, .	7.2	17
2183	Noncovalent Interactions in the Oxazaborolidine-Catalyzed Enantioselective Mukaiyama Aldol. Journal of Organic Chemistry, 2022, 87, 10054-10061.	1.7	1
2184	Valeriana pilosa Roots Essential Oil: Chemical Composition, Antioxidant Activities, and Molecular Docking Studies on Enzymes Involved in Redox Biological Processes. Antioxidants, 2022, 11, 1337.	2.2	5
2185	Synthesis, characterization and self assembly of dinuclear zinc Schiff base complexes: A combined experimental and theoretical study. Polyhedron, 2022, 225, 116044.	1.0	5
2186	Excess properties, spectral analysis and computational chemistry of (1,3-propanediolÂ+Âethylenediamine) ion-like liquids for CS2 capture. Journal of Molecular Liquids, 2022, 363, 119830.	2.3	9
2187	Hydrocarbon Soluble Alkaliâ€Metalâ€Aluminium Hydride Surrog[ATES]. Chemistry - A European Journal, 2022, 28, .	1.7	9
2188	Cation <mml:math <br="" xmlns:mml="http://www.w3.org/1998/Math/MathML">altimg="si74.svg"&gt;<mml:mrow><mml:mo>â&lt;¯</mml:mo></mml:mrow></mml:math> anion bonding interactions in 1–Ethyl–3–Methylimidazolium based ionic liquids. Chemical Physics, 2022, 562, 111648.	0.9	1

#	Article	IF	CITATIONS
2189	Molecular dynamics study of water and ion behaviors of mixed salts solutions on extended quartz surface. Journal of Applied Physics, 2022, 132, 024701.	1.1	0
2190	Desymmetrization of N-Cbz glutarimides through N-heterocyclic carbene organocatalysis. Nature Communications, 2022, 13, .	5.8	12
2191	DFT study on CHâ<¯O, CH···SCN and SÂ·Â·Â ï€ interaction energies in three dinuclear mixed valence cobalt(III/II complexes with secondary diamine ligands having inner N2O2 and outer O4 compartments. Polyhedron, 2022, , 116039.	) 1.0	1
2192	Allosteric enhancement of the BCR-Abl1 kinase inhibition activity of nilotinib by cobinding of asciminib. Journal of Biological Chemistry, 2022, 298, 102238.	1.6	13
2193	Extraction of flavonoids from Glycyrrhiza residues using deep eutectic solvents and its molecular mechanism. Journal of Molecular Liquids, 2022, 363, 119848.	2.3	18
2194	Supramolecular assemblies involving unconventional non-covalent contacts in pyrazole-based coordination compounds of Co(II) and Cu(II) pyridinedicarboxylates: Antiproliferative evaluation and theoretical studies. Polyhedron, 2022, 224, 116025.	1.0	2
2195	Sumanene as a delivery carrier for methimazole drug: DFT, AIM, SERS and solvent effects. Computational and Theoretical Chemistry, 2022, 1215, 113811.	1.1	16
2196	Structural elucidation of phenoxybenzaldehyde derivatives from laboratory powder X-ray diffraction: A combined experimental and theoretical quantum mechanical study. Journal of Molecular Structure, 2022, 1268, 133697.	1.8	14
2197	A Ni(II) chetale of an unsymmetrical N2O3 donor ligand and its use as flexidentate metalloligand to synthesise heterometallic Ni(II)-Mn(II) complexes: recurrent CH··΀ and π-stacking motifs in the structures. Inorganica Chimica Acta, 2022, , 121111.	1.2	1
2198	Dispersion Stabilizes Metal–Metal Bonds in the 1,8-Bis(silylamido)naphthalene Ligand Environment. Organometallics, 2022, 41, 2180-2187.	1.1	6
2199	Molecular Electrides: An In Silico Perspective. ChemPhysChem, 2022, 23, .	1.0	4
2200	Adsorption of Pesticides, Antibiotics and Microcystin-LR by Graphene and Hexagonal Boron Nitride Nano-Systems: A Semiempirical PM7 and Theoretical HSAB Study. Crystals, 2022, 12, 1068.	1.0	3
2201	Unravelling the Synthetic Mimic, Spectroscopic Insights, and Supramolecular Crystal Engineering of an Innovative Heteronuclear Pb(II)-Salen Cocrystal: An Integrated DFT, QTAIM/NCI Plot, NLO, Molecular Docking/PLIP, and Antibacterial Appraisal. Journal of Inorganic and Organometallic Polymers and Materials, 2022, 32, 4320-4339.	1.9	19
2202	The tetrel bonding role in supramolecular aggregation of lead(II) acetate and a thiosemicarbazide derivative. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 685-694.	0.5	5
2203	In silico study of tacrine and acetylcholine binding profile with human acetylcholinesterase: docking and electronic structure. Journal of Molecular Modeling, 2022, 28, .	0.8	6
2204	Initial recognition and attachment of the Zika virus to host cells: A molecular dynamics and quantum interaction approach. ChemBioChem, 0, , .	1.3	4
2205	Noncovalent interactions between benzochalcogenadiazoles and nitrogen bases. Journal of Molecular Modeling, 2022, 28, .	0.8	4
2206	Photoâ€Oxidizing Ruthenium(II) Complexes with Enhanced Visibleâ€Light Absorption and Gâ€quadruplex DNA Binding Abilities. Chemistry - A European Journal, 2022, 28, .	1.7	5

#	Article	IF	CITATIONS
2207	Halogen··À·Halogen and ï€â€"Hole Interactions in Supramolecular Aggregates and Electrical Conductivity Properties of Cu(II)-Based 1D Coordination Polymers. Crystal Growth and Design, 2022, 22, 5189-5197.	1.4	13
2208	Selenium(IV) Polybromide Complexes: Structural Diversity Driven by Halogen and Chalcogen Bonding. Molecules, 2022, 27, 5355.	1.7	2
2209	Is the phosphorous atom a stereogenic center? Crystallographic findings in five new dithiophosphonate compounds supported with non covalent interaction index (NCI), theoretical approach and spectroscopic analysis. Journal of Molecular Structure, 2022, 1270, 133987.	1.8	1
2210	Ir and NHC Dual Chiral Synergetic Catalysis: Mechanism and Stereoselectivity in Î <sup>3</sup> -Butyrolactone Formation. Journal of the American Chemical Society, 2022, 144, 16171-16183.	6.6	14
2211	Nonbonded Force Field Parameters from Minimal Basis Iterative Stockholder Partitioning of the Molecular Electron Density Improve CB7 Host–Guest Affinity Predictions. Journal of Chemical Information and Modeling, 2022, 62, 4162-4174.	2.5	1
2212	Influence of 5-Halogenation on the Base-Pairing Energies of Protonated Cytidine Nucleoside Analogue Base Pairs: Implications for the Stabilities of Synthetic <i>i</i> Motif Structures for DNA Nanotechnology Applications. Journal of the American Society for Mass Spectrometry, 0, , .	1.2	1
2213	Microhydration of Phenyl Formate: Gasâ€Phase Laser Spectroscopy, Microwave Spectroscopy, and Quantum Chemistry Calculations. ChemPhysChem, 0, , .	1.0	2
2214	Selective separation of light rare-earth elements by supramolecular encapsulation and precipitation. Nature Communications, 2022, 13, .	5.8	19
2215	Liquid–liquid equilibrium measurements and computational study of salt–polymer aqueous two phase system for extraction of analgesic drugs. Scientific Reports, 2022, 12, .	1.6	4
2216	Search for Novel Potent Inhibitors of the SARS-CoV-2 Papain-like Enzyme: A Computational Biochemistry Approach. Pharmaceuticals, 2022, 15, 986.	1.7	1
2217	DFT rationalization of metal-catalyst-controlled coupling of carbazole with diazo-naphthalen-2(1H)-one. Molecular Catalysis, 2022, 529, 112574.	1.0	1
2218	Bidentate Rh(I)â€Phosphine Complexes for the Câ <sup>~</sup> H Activation of Alkanes: Computational Modelling and Mechanistic Insight. ChemCatChem, 2022, 14, .	1.8	1
2219	Lewis Superacidic Divalent Bis( <i>m</i> â€ŧerphenyl)element Cations [(2,6â€Mes <sub>2</sub> C <sub>6</sub> H <sub>3</sub> ) <sub>2</sub> E] <sup>+</sup> of Group 13 Revisited and Extended (E=B, Al, Ga, In, Tl). European Journal of Inorganic Chemistry, 2023, 26, .	1.0	2
2220	London Dispersion Stabilizes Chloro-Substituted cis-Double Bonds. Synlett, 2023, 34, 1129-1134.	1.0	2
2221	Understanding the Kinetics and Topological Events Within the Thioneâ€ŧoâ€īhiol Rearrangement of Xanthates. ChemistrySelect, 2022, 7, .	0.7	1
2222	Microsolvation versus encapsulation in mono, di, and trivalent cations. ChemPhysChem, 0, , .	1.0	2
2223	NHC-catalyzed [3Â+Â4] annulation between 2-dromoenal and aryl 1,2-diamine: Insights into mechanisms, chemo and stereoselectivities. Molecular Catalysis, 2022, 530, 112604.	1.0	1
2224	A comparative study of the potential energy surfaces of (CO)2, CO-CS and (CS)2. Computational and Theoretical Chemistry, 2022, 1215, 113849.	1.1	2

#	Article	IF	CITATIONS
2225	Adsorption of glyphosate on graphene and functionalized graphenes: A DFT study. Computational and Theoretical Chemistry, 2022, 1215, 113840.	1.1	0
2226	Bromochlorodifluoromethane interaction with pristine and doped BN nanosheets: A DFT study. Journal of Environmental Chemical Engineering, 2022, 10, 108367.	3.3	13
2227	Surface functionalization of Si6Li6 cluster with superalkalis to achieve high nonlinear optical response: A DFT study. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 653, 129985.	2.3	7
2228	Insight into the cation-regulated mechanism for the hydration of propargyl alcohols catalyzed by [Bu4P+][Imâ^']. Journal of Molecular Liquids, 2022, 365, 120021.	2.3	1
2229	New complexes of indium(III) diaryldithiophosphates: Structural characterization and insight into supramolecular interactions. Polyhedron, 2022, 226, 116094.	1.0	4
2230	Exploring dithiolate-amine binary ligand systems for the supramolecular assemblies of Ni(II) coordination compounds: Crystal structures, theoretical studies, cytotoxicity studies, and molecular docking studies. Inorganica Chimica Acta, 2022, 543, 121157.	1.2	3
2231	Quantum Chemical Approach to the Adsorption of Chlorpyrifos and Fenitrothion on the Carbon-Doped Boron Nitride Nanotube Decorated with Tetrapeptide. Crystals, 2022, 12, 1285.	1.0	1
2232	Spectroscopic studies of 5-fluoro-1H-pyrimidine-2,4-dione adsorption on nanorings, solvent effects and SERS analysis. Computational and Theoretical Chemistry, 2022, 1217, 113873.	1.1	2
2233	Water-dispersible polymer coated silica nanoparticle for turn-on fluorometric detection of Cephalexin. Biosensors and Bioelectronics: X, 2022, 12, 100231.	0.9	0
2234	Investigation of the adsorption of a DNA based purine derivative on N/B-doped coronene and coronene by means of DFT and NCI interaction analysis. Journal of Molecular Liquids, 2022, 367, 120373.	2.3	12
2235	Synthesis, structural characterization, DNA interaction, dye adsorption properties and theoretical studies of copper (II) carboxylates. Journal of Molecular Structure, 2023, 1272, 134104.	1.8	4
2236	Heterovalent chalcogen bonding: supramolecular assembly driven by the occurrence of a tellurium( <scp>ii</scp> )â< Ch( <scp>i</scp> ) (Ch = S, Se, Te) linkage. Inorganic Chemistry Frontiers, 2022, 9, 5635-5644.	3.0	5
2237	Deciphering the Cooperative Effect of Base and N-Substituents on the Origin of Regioselectivity Switching for Mannich Reactions of Glycinate by Carbonyl Catalysts. SSRN Electronic Journal, 0, , .	0.4	0
2238	Fumarato and phthalato bridged dinuclear metal–organic Cu( <scp>ii</scp> ) and Mn( <scp>ii</scp> ) compounds involving infinite fumarate–water assemblies and unusual structure-guiding H-bonded synthons: antiproliferative evaluation and theoretical studies. New Journal of Chemistry, 2022, 46, 17817-17833.	1.4	0
2239	A solvent-mediated conformational switch in sulfanilamide. Physical Chemistry Chemical Physics, 2022, 24, 24032-24038.	1.3	2
2240	Unravelling the binding affinity and selectivity of molybdenum( <scp>ii</scp> ) phenanthroline complexes with DNA G-quadruplexes by using linear-scaling DFT studies. The important role of ancillary ligands. Physical Chemistry Chemical Physics, 2022, 24, 25918-25929.	1.3	3
2241	On the importance of π-stacking interactions in the complexes of copper and zinc bearing pyridine-2,6-dicarboxylic acid <i>N</i> -oxide and N-donor auxiliary ligands. CrystEngComm, 2022, 24, 6677-6687.	1.3	2
2242	Importance of Cu and Ag regium–π bonds in supramolecular chemistry and biology: a combined crystallographic and <i>ab initio</i> study. Physical Chemistry Chemical Physics, 2022, 24, 24983-24991.	1.3	3

#	Article	IF	CITATIONS
2243	Efficient fluorescent recognition of ATP/GTP by a water-soluble bisquinolinium pyridine-2,6-dicarboxamide compound. Crystal structures, spectroscopic studies and interaction mode with DNA. RSC Advances, 2022, 12, 27826-27838.	1.7	3
2244	Ni( <scp>i</scp> )–TPA stabilization by hydrogen bond formation on the second coordination sphere: a DFT characterization. Dalton Transactions, 2022, 51, 12585-12595.	1.6	3
2245	Exploiting the "Lego brick―approach to predict accurate molecular structures of PAHs and PANHs. Physical Chemistry Chemical Physics, 2022, 24, 23254-23264.	1.3	13
2246	<i>In silico</i> activation of dinitrogen with a light atom molecule. Physical Chemistry Chemical Physics, 2022, 24, 20953-20967.	1.3	3
2247	The <i>N</i> , <i>N</i> , <i>N</i> -trimethylammonium moiety as tetrel bond donor site: crystallographic and computational studies. Physical Chemistry Chemical Physics, 2022, 24, 24892-24901.	1.3	2
2248	Identification of 4-acrylamido- <i>N</i> -(pyridazin-3-yl)benzamide as anti-COVID-19 compound: a DFTB, molecular docking, and molecular dynamics study. RSC Advances, 2022, 12, 24178-24186.	1.7	3
2249	Computational modeling and characterization of secondary bonding in compounds of late p-block elements. , 2022, , .		0
2250	Unprecedented {d <sub><i>z</i><sup>2</sup></sub> -Cu <sup>II</sup> O <sub>4</sub> }â<'ï€-hole interactions: the case of a cocrystal of a Cu( <scp>ii</scp> ) bis-î²-diketonate complex with 1,4-diiodotetrafluoro-benzene. Chemical Communications, 2022, 58, 9524-9527.	2.2	3
2251	γ-Agostic interactions in ( <sup>Mes</sup> CCC)Fe–Mes(L) complexes. Chemical Communications, 2022, 58, 9626-9629.	2.2	5
2252	2-Picolinic acid as a naturally occurring hydrogen bond donor for the preparation of cyclic carbonates from terminal/internal epoxides and CO <sub>2</sub> . Green Chemistry, 2022, 24, 9069-9083.	4.6	11
2253	<i>In silico</i> capture of noble gas atoms with a light atom molecule. Physical Chemistry Chemical Physics, 2022, 24, 20968-20979.	1.3	2
2254	Crystal engineering of molecules with through-space α-effect hydrogen bonds: 3a,6 : 7,9a-diepoxybenzo[ <i>de</i> ]isoquinolines possessing a free amino group. CrystEngComm, 2022, 6093-6100.	243	0
2255	Time-dependent density functional theory studies of the optical and electronic properties of the [M <sub>25</sub> (MPA) <sub>18</sub> ] <sup>â^'</sup> (M = Au, Ag, MPA =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 24457-24468.	50 262 Td 1.3	(SCH <sub></sub>
2256	Insight into non-covalent interactions in 1D Gd-based coordination polymer for solid-state self-assembly through a new supramolecular synthon. Journal of Molecular Structure, 2023, 1272, 134204.	1.8	4
2257	Ultra-sensitive fluorescent and colorimetric probes for femtomolar detection of picric acid: Mechanochromic, latent fingerprinting, and pH responsive character with AIE properties. Journal of Photochemistry and Photobiology A: Chemistry, 2023, 435, 114318.	2.0	13
2258	Ultralong C(sp3)–C(sp3) Single Bonds Shortened and Stabilized by London Dispersion. Synlett, 2023, 34, 1147-1152.	1.0	2
2259	Isocyanide and Cyanide Entities Form Isostructural Halogen Bond-Based Supramolecular Networks Featuring Five-Center Tetrafurcated Halogen···C/N Bonding. Crystal Growth and Design, 2022, 22, 6079-6087.	1.4	8
2260	Theoretical Analysis of the Adsorption of Pentachlorophenol and 6-OH-BDE-47 (6-Hydroxy-2,2',4,4'-Tetrabromodiphenyl Ether) by Boron Nitride Nanotubes Decorated with Double-Decker Lanthanide(III) Phthalocyanine Complexes. Crystals, 2022, 12, 1205.	1.0	0

#	Article	IF	CITATIONS
2261	Binding Energy Partition of Promising IRAKâ€4 Inhibitor (Zimlovisertib) for the Treatment of COVIDâ€19 Pneumonia. ChemPhysChem, 2022, 23, .	1.0	1
2262	Silyl Groups Are Strong Dispersion Energy Donors. Journal of Organic Chemistry, 2022, 87, 13168-13177.	1.7	5
2263	Synthesis and Crystallographic Characterisation of Pyridyl- and Indoleninyl-Substituted Pyrimido[1,2-b]Indazoles. Crystals, 2022, 12, 1283.	1.0	3
2264	Spectroscopic Studies of Styrylquinoline Copolymers with Different Substituents. Polymers, 2022, 14, 4040.	2.0	1
2265	A pocket-based 3D molecule generative model fueled by experimental electron density. Scientific Reports, 2022, 12, .	1.6	8
2266	Theoretical study of the interaction of fullerenes with the emerging contaminant carbamazepine for detection in aqueous environments. Scientific Reports, 2022, 12, .	1.6	6
2267	Theoretical study of glycoluril by highly symmetrical magnesium oxide Mg12O12 nanostructure: adsorption, detection, SERS enhancement, and electrical conductivity study. Journal of Molecular Modeling, 2022, 28, .	0.8	6
2268	Aryldiazonium salts can serve as nitrogen-based Lewis acid catalysts and their applications in the formation of photoactive charge transfer complexes. Chinese Chemical Letters, 2023, 34, 107821.	4.8	4
2269	Tris(2-Pyridyl)Arsine as a New Platform for Design of Luminescent Cu(I) and Ag(I) Complexes. Molecules, 2022, 27, 6059.	1.7	10
2270	GCMC and electronic evaluation of pesticide capture by IRMOF systems. Journal of Molecular Modeling, 2022, 28, .	0.8	1
2271	Thermodynamic and Computational (DFT) Study of Non-Covalent Interaction Mechanisms of Charge Transfer Complex of Linagliptin with 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) and Chloranilic acid (CHA). Molecules, 2022, 27, 6320.	1.7	10
2272	Exploring of spacer fluorination effect on the characteristics and physicochemical properties of the newly designed task specific dicationic imidazolium-based ionic liquids: A quantum chemical approach. Journal of Fluorine Chemistry, 2022, 261-262, 110026.	0.9	3
2273	OH <sup>–</sup> ···Au Hydrogen Bond and Its Effect on the Oxygen Reduction Reaction on Au(100) in Alkaline Media. Journal of Physical Chemistry Letters, 2022, 13, 9035-9043.	2.1	1
2274	Unveiling the Shape of <i>N</i> -Acetylgalactosamine: A Cancer-Associated Sugar Derivative. Journal of Physical Chemistry A, 2022, 126, 7621-7626.	1.1	1
2275	Crystallographic and Theoretical Study of Osme Bonds in Nitrido-Osmium(VI) Complexes. Inorganics, 2022, 10, 133.	1.2	4
2276	Computational Study on the Co-Mediated Intramolecular Pauson–Khand Reaction of Fluorinated and Chiral <i>N</i> -Tethered 1,7-Enynes. Organometallics, 2022, 41, 2525-2534.	1.1	3
2277	Facile Access to 2-Selenoxo-1,2,3,4-tetrahydro-4-quinazolinone Scaffolds and Corresponding Diselenides via Cyclization between Methyl Anthranilate and Isoselenocyanates: Synthesis and Structural Features. Molecules, 2022, 27, 5799.	1.7	4
2278	Unraveling the Role of the Tyrosine Tetrad from the Binding Site of the Epigenetic Writer MLL3 in the Catalytic Mechanism and Methylation Multiplicity. International Journal of Molecular Sciences, 2022, 23, 10339.	1.8	2

#	Article	IF	CITATIONS
2279	Structural and Energetic Properties of Weak Noncovalent Interactions in Two Closely Related 3,6-Disubstituted-[1,2,4]triazolo[3,4- <i>b</i> ][1,3,4]thiadiazole Derivatives: In Vitro Cyclooxygenase Activity, Crystallography, and Computational Investigations. ACS Omega, 2022, 7, 34506-34520.	1.6	2
2280	An Iridium-Stabilized Borenium Intermediate. Journal of the American Chemical Society, 2022, 144, 18359-18374.	6.6	11
2281	Stacking Interactions: A Supramolecular Approach to Upgrade Weak Halogen Bond Donors. Chemistry - A European Journal, 2022, 28, .	1.7	9
2282	An insight into interaction of the uracil, thymine and cytosine biomolecules with methimazole anti-thyroid drug: DFT and GD3‑DFT approaches. Structural Chemistry, 0, , .	1.0	2
2283	Inâ€silico exploration of noble gas dimer enforced by noncovalent interaction. International Journal of Quantum Chemistry, 2023, 123, .	1.0	3
2284	Halogen or Arene: Complexation of 4,4'-Dibromobiphenyl with a Trinuclear Silver(I) Macrocycle. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2022, 48, 615-621.	0.3	0
2285	Synthesis and Xâ€ray Characterization of 4,5â€Dihydropyrazolylâ€Thiazoles Bearing a Coumarin Moiety: On the Importance of Antiparallel Ï€â€Stacking. ChemistrySelect, 2022, 7, .	0.7	8
2286	Bi- or trinuclear 2-iodobenzoate complexes of Znii: crystal structures and luminescence. Mendeleev Communications, 2022, 32, 585-587.	0.6	1
2287	Polymorph-Dependent Phosphorescence of Cyclometalated Platinum(II) Complexes and Its Relation to Non-covalent Interactions. ACS Omega, 2022, 7, 34454-34462.	1.6	11
2288	Expanding the Knowledge of the Selective-Sensing Mechanism of Nitro Compounds by Luminescent Terbium Metal–Organic Frameworks through Multiconfigurational <i>ab Initio</i> Calculations. Journal of Physical Chemistry A, 2022, 126, 7040-7050.	1.1	8
2289	Detailed Density Functional Theory Study of the Cationic Zirconocene Compound [Cp(C <sub>5</sub> H <sub>4</sub> CMe <sub>2</sub> C <sub>6</sub> H <sub>4</sub> F)ZrMe] <sup>+</sup> . ACS Omega, 2022, 7, 35136-35152.	1.6	1
2290	Noncovalent Stabilization of Radical Intermediates in the Enantioselective Hydroamination of Alkenes with Sulfonamides. Journal of the American Chemical Society, 2022, 144, 18948-18958.	6.6	11
2291	New task-specific ionic liquids based on phenyl diazenyl methyl pyridinium cation: Energetic, electronic and optical properties exploration based on DFT calculations. Journal of Molecular Graphics and Modelling, 2023, 118, 108352.	1.3	2
2292	Effect of Propargylic Substituents on Enantioselectivity and Reactivity in Ruthenium-Catalyzed Propargylic Substitution Reactions: A DFT Study. ACS Omega, 2022, 7, 36634-36642.	1.6	3
2293	Supramolecular and theoretical investigation of copper(II) complexes containing 2,2′-bipyridine and substituted chalcone ligands: Estimation of non-covalent interactions. Journal of Molecular Structure, 2023, 1273, 134271.	1.8	4
2294	Influence of HSA on micellization of NLSS and BC: An experimental-theoretical approach of its binding characteristics. Journal of Molecular Liquids, 2022, 367, 120532.	2.3	4
2295	Deciphering the cooperative effect of base and N-substituents on the origin of enantioselectivity switching for Mannich reactions of glycinate by carbonyl catalysts. Journal of Catalysis, 2022, 415, 1-11.	3.1	4
2296	DFT, solvation effects, reactivity and SERS analysis on structural, optical, and vibrational properties of a biomolecule of pyrimidine derivative adsorbed on metal clusters of Ag/Au/Cu. Journal of the Indian Chemical Society, 2022, 99, 100753.	1.3	9

#	Article	IF	CITATIONS
2297	An efficient initiator system containing AlCl3 and supported ionic-liquid for the synthesis of conventional grade polyisobutylene in mild conditions. Journal of Molecular Liquids, 2022, 367, 120381.	2.3	12
2298	Load-bearing study and interfacial interactions of hydroxyapatite composite coatings for bone tissue engineering. Materials Chemistry Frontiers, 2022, 6, 3731-3747.	3.2	8
2299	Mechanism of [3+2] Annulations between Indole-2-formaldehydes and Isatins Mediated by N-Heterocyclic Carbene: A DFT Study. New Journal of Chemistry, 0, , .	1.4	0
2300	The many forms of alpha-methoxy phenylacetic acid in the gas phase: flexibility, internal dynamics, and their intramolecular interactions. Physical Chemistry Chemical Physics, 2022, 24, 27312-27320.	1.3	1
2301	Dual-Ligand Strategy Employing Rigid 2,5-Thiophenedicarboxylate and 1,10-Phenanthroline as Coligands for Solvothermal Synthesis of Eight Lanthanide(III) Coordination Polymers: Structural Diversity, DFT Study, and Exploration of the Luminescent Tb(III) Coordination Polymer as an Efficient Chemical Sensor for Nitroaromatic Compounds. ACS Omega, 2022, 7, 41370-41391.	1.6	9
2302	Covalent Organic Framework (C6N6) as a Drug Delivery Platform for Fluorouracil to Treat Cancerous Cells: A DFT Study. Materials, 2022, 15, 7425.	1.3	15
2303	Studies on the Interaction of Rose Bengal with the Human Serum Albumin Protein under Spectroscopic and Docking Simulations Aspects in the Characterization of Binding Sites. Chemosensors, 2022, 10, 440.	1.8	2
2304	Stereochemistry Controls Dihydrogen Bonding Strengths in Chiral Amine Boranes Adducts. Angewandte Chemie - International Edition, 2022, 61, .	7.2	2
2305	Stereochemistry Controls Dihydrogen Bonding Strengths in Chiral Amine Boranes Adducts. Angewandte Chemie, 0, , .	1.6	0
2306	Matere Bonds vs. Multivalent Halogen and Chalcogen Bonds: Three Case Studies. Molecules, 2022, 27, 6597.	1.7	13
2307	Dicationic ionic liquids (DILs) based on the phenyl and perfluoro-phenyl π-spacer-linked triazolium cations: a quantum chemical comparative study. Theoretical Chemistry Accounts, 2022, 141, .	0.5	3
2308	Characterization of a Ferryl Flip in Electronically Tuned Nonheme Complexes. Consequences in Hydrogen Atom Transfer Reactivity. Angewandte Chemie, 0, , .	1.6	0
2309	Dicarboxylic Acid-Based Co-Crystals of Pyridine Derivatives Involving Structure Guiding Unconventional Synthons: Experimental and Theoretical Studies. Crystals, 2022, 12, 1442.	1.0	1
2310	DFT study of therapeutic potential of graphitic carbon nitride as a carrier for controlled release of melphalan: an anticancer drug. Journal of Molecular Modeling, 2022, 28, .	0.8	3
2311	Atropodiastereoselective 5 <i>N</i> -Acylation of 1,5-Benzodiazepin-2-ones with ( <i>S</i> )-2-Phenylpropanoyl and ( <i>S</i> )-2-Phenylbutanoyl Chlorides. Journal of Organic Chemistry, 2022, 87, 15289-15300.	1.7	1
2312	Mechanistic Insights into Cobalt-Catalyzed Regioselective C4-Alkenylation of 3-Acetylindole: A Detailed Theoretical Study. Journal of Organic Chemistry, 2022, 87, 14125-14136.	1.7	1
2313	DFT analysis on the adsorption of melamine in Ga <sub>12</sub> -N <sub>12</sub> /P <sub>12</sub> nanocages: solvent effects, SERS analysis, reactivity properties. Journal of Biomolecular Structure and Dynamics, 2023, 41, 8844-8855.	2.0	4
2314	Characterization of a Ferryl Flip in Electronically Tuned Nonheme Complexes. Consequences in Hydrogen Atom Transfer Reactivity. Angewandte Chemie - International Edition, 2023, 62, .	7.2	4

#	Article	IF	CITATIONS
2315	Identifying the role of excitedâ€state proton transfer and photoinduced electron transfer in detecting hypochlorous acid for a benzothiazoleâ€based colorimetric fluorescent probe. Journal of Physical Organic Chemistry, 2023, 36, .	0.9	2
2316	Carboxylic Acid Directed γ-Lactonization of Unactivated Primary C–H Bonds Catalyzed by Mn Complexes: Application to Stereoselective Natural Product Diversification. Journal of the American Chemical Society, 2022, 144, 19542-19558.	6.6	26
2317	Effect of the Silica–Magnetite Nanocomposite Coating Functionalization on the Doxorubicin Sorption/Desorption. Pharmaceutics, 2022, 14, 2271.	2.0	7
2318	Complexes of carbon dioxide with methanol and its monohalogen-substituted: beyond the tetrel bond. Chemical Physics Letters, 2022, , 140158.	1.2	2
2319	Stimulation calculation of desulfurization mechanisms dominated by free radicals reactions during pyrolysis of thiophenes under water vapor atmosphere. Computational and Theoretical Chemistry, 2022, 1217, 113912.	1.1	0
2320	Formation of C60-SnI4 Adducts. Insights of the role of $lf$ -hole and Tetrel-bonding in the Strength and Interaction Nature from DFT calculations. Inorganica Chimica Acta, 2022, , 121277.	1.2	0
2321	Modeling of pristine, Ir- and Au-decorated C60 fullerenes as sensors for detection of hydroxyurea and nitrosourea drugs. Journal of Environmental Chemical Engineering, 2022, 10, 108802.	3.3	40
2322	Be doped carbon nanoring for hydrogen storage using density functional theory. Journal of Energy Storage, 2022, 56, 105979.	3.9	3
2323	Molecular electrides: An overview of their structure, bonding, and reactivity. , 2023, , 275-295.		0
2324	Quantitative analysis of intermolecular interactions in crystalline substituted triazoles. Journal of Molecular Structure, 2023, 1273, 134380.	1.8	3
2325	A study on the catalytic activity of polypeptides toward the hydrolysis of glucoside compounds gastrodin, polydatin and esculin. Journal of Materials Chemistry B, 2022, 10, 9878-9886.	2.9	1
2326	Comparative oxidative ability of mononuclear and dinuclear high-valent iron–oxo species towards the activation of methane: does the axial/bridge atom modulate the reactivity?. Dalton Transactions, 2023, 52, 308-325.	1.6	3
2327	Spectroscopic, reactivity analysis and docking studies of 3-(adamantan-1-yl)-4-(4-fluorophenyl)-1-[(4-phenylpiperazin-1-yl)methyl]-4,5-dihdyro-1H-1,2,4-triazole—5-thione: DFT and MD simulations. Journal of Molecular Structure, 2023, 1274, 134418.	1.8	3
2328	Supramolecular assemblies involving energetically significant unconventional π(CN)-π and anion-Ï€(nitrile) contacts in Zn(II) coordination compounds: Antiproliferative evaluation and theoretical studies. Journal of Molecular Structure, 2023, 1274, 134568.	1.8	2
2329	Unusual Changes of C–H Bond Lengths in Chiral Zinc Complexes Induced by Noncovalent Interactions. Angewandte Chemie, 0, , .	1.6	0
2330	In silico investigation of organometallic complexes for identification of RNase A inhibitor. Journal of Organometallic Chemistry, 2023, 983, 122556.	0.8	3
2331	Novel Organotin(IV) Complexes of 2-[4-Hydroxy-3-((2-hydroxyethylimino)methyl)phenylazo]benzoic Acid: Synthesis, Structure, Noncovalent Interactions and In Vitro Antibacterial Activity. Crystals, 2022, 12, 1582.	1.0	10
2332	Absorption spectra of calix[3]pyrrole analogs as probes for contracted macrocycles. Journal of Porphyrins and Phthalocyanines, 0, , .	0.4	2

#	Article	IF	CITATIONS
2333	Exploring Solid‣tate Supramolecular Architectures of Penta(carboxymethyl)diethylenetriamine: Experimental Observation and Theoretical Studies. ChemistrySelect, 2022, 7, .	0.7	8
2334	Designing neodymium-doped hexamine complexant as novel IR NLO material with extremely large non-linear optical behavior. Journal of Molecular Modeling, 2022, 28, .	0.8	1
2335	Unusual Changes of C–H Bond Lengths in Chiral Zinc Complexes Induced by Noncovalent Interactions. Angewandte Chemie - International Edition, 0, , .	7.2	2
2336	The essential oil from Drimys winteri possess activity: Antioxidant, theoretical chemistry reactivity, antimicrobial, antiproliferative and chemical composition. , 0, 1, .		0
2337	Study on Gas Chromatography Retention Time Variation of Acetic Acid Combined with Quantum Chemical Calculation. Chromatographia, 2023, 86, 3-11.	0.7	1
2338	Nature and role of formal charge of the ion inclusion in hexanuclear Platinum(II) Host-Guest Species. Insights from relativistic DFT calculations. Inorganica Chimica Acta, 2023, 546, 121298.	1.2	2
2339	Automated and Efficient Generation of General Molecular Aggregate Structures. Angewandte Chemie - International Edition, 2023, 62, .	7.2	11
2340	Halogenation of the 3-position of pyridines through Zincke imine intermediates. Science, 2022, 378, 773-779.	6.0	35
2341	Beryllium bonding with noble gas atoms. Journal of Computational Chemistry, 2023, 44, 644-655.	1.5	2
2342	Automated and Efficient Generation of General Molecular Aggregate Structures. Angewandte Chemie, 2023, 135, .	1.6	3
2344	Theoretical Study on Spectrum and Luminescence Mechanism of Indocyanine Green Dye Based on Density Functional Theory (DFT). Journal of Chemistry, 2022, 2022, 1-8.	0.9	1
2345	Structure and conformations of 3-methylcatechol: A rotational spectroscopic and theoretical study. Journal of Molecular Spectroscopy, 2022, 390, 111715.	0.4	3
2346	Role of O–Hâ<¯O/S conventional hydrogen bonds in considerable C <sub>sp<sup>2</sup></sub> –H blue-shift in the binary systems of acetaldehyde and thioacetaldehyde with substituted carboxylic and thiocarboxylic acids. RSC Advances, 2022, 12, 35309-35319.	1.7	1
2347	Towards predictive computational catalysis – a case study of olefin metathesis with Mo imido alkylidene N-heterocyclic carbene catalysts. Chemical Modelling, 2022, , 1-23.	0.2	1
2348	Exploration of Cl⋯Cl and π⋯i€ stacking contacts along with the conductivity properties of a Cu-MOF featured with paddle-wheel SBUs. CrystEngComm, 2023, 25, 813-821.	1.3	1
2349	Revealing the supramolecular features of two Zn( <scp>ii</scp> ) complexes derived from a new hydrazone ligand: a combined crystallographic, theoretical and antibacterial study. CrystEngComm, 2023, 25, 866-876.	1.3	1
2350	Synthesis, structural characterization and DFT study of <i>N</i> -(pyrimidyl)-ω-amino acids/peptide: β-alanine, γ-aminobutyric acid, 5-aminovaleric acid, 6-aminohexanoic acid and glycylglycine. CrystEngComm, 0, , .	1.3	0
2351	${ m i} f$ -Hole triel bonds in aluminium derivatives. Dalton Transactions, 2023, 52, 551-555.	1.6	2

#	Article	IF	CITATIONS
2352	Theoretical investigation of intermolecular interactions between CNT, SiCNT and SiCGeNT nanomaterials with vinyl chloride molecule: A DFT, NBO, NCI, and QTAIM study. Diamond and Related Materials, 2023, 131, 109602.	1.8	7
2353	Enclathration of Mn(II)(H2O)6 guests and unusual Cuâ< O bonding contacts in supramolecular assemblies of Mn(II) Co-crystal hydrate and Cu(II) Pyridinedicarboxylate: Antiproliferative evaluation and theoretical studies. Polyhedron, 2023, 230, 116243.	1.0	2
2354	π–π stacking in the polymorphism of 2-(naphthalenylamino)-nicotinic acids and a comparison with their analogues. CrystEngComm, 2023, 25, 432-443.	1.3	1
2355	Mono-anionic succinic acid bridged cationic cobalt(III/II/III) compounds of N2O2 donor â€~reduced Schiff base' ligands containing perchlorate counter ions: Synthesis, structures and different non-covalent interactions in self-assembly. Results in Chemistry, 2023, 5, 100701.	0.9	0
2356	A ratiometric fluorescent sensor based on metalloenzyme mimics for detecting organophosphorus pesticides. Sensors and Actuators B: Chemical, 2023, 377, 133031.	4.0	6
2357	High drug carrying efficiency of boron-doped Triazine based covalent organic framework toward anti-cancer tegafur; a theoretical perspective. Computational and Theoretical Chemistry, 2023, 1220, 113990.	1.1	18
2358	Adsorbing CNCl on pristine, C-, and Al-doped boron nitride nanotubes: A density functional theory study. Computational and Theoretical Chemistry, 2023, 1220, 113980.	1.1	7
2359	Dihydrolevoglycosenone as a novel bio-based nanofluid for thermal energy storage: Physiochemical and quantum chemical insights. Journal of Energy Storage, 2023, 59, 106365.	3.9	5
2360	Crystal engineering of Pb(II)-salen coordination polymer enforced for the selective fluorescence NACs sensing activity in a dispersed aqueous medium: A combined experimental and theoretical DFT monologue. Journal of Molecular Structure, 2023, 1276, 134717.	1.8	9
2361	An insight to the role of perchlorate counter ions and different non-covalent interactions in the solid state structures of mono-anionic malonic acid bridged trinuclear mixed valence cationic complexes of cobalt with tetradentate N2O2 donor ligands. Inorganica Chimica Acta, 2023, 547, 121324.	1.2	4
2362	The importance of tetrel bonding interactions with carbon in two arrestive iso-structural Cd( <scp>ii</scp> )–Salen coordination complexes: a comprehensive DFT overview in crystal engineering. RSC Advances, 2022, 12, 35860-35872.	1.7	4
2363	DFT and COSMO-RS studies on dicationic ionic liquids (DILs) as potential candidates for CO <sub>2</sub> capture: the effects of alkyl side chain length and symmetry in cations. RSC Advances, 2022, 12, 35418-35435.	1.7	2
2364	Cu(II)-Based Molecular Hexagons Forming Honeycomb-like Networks Exhibit High Electrical Conductivity. Inorganic Chemistry, 2022, 61, 19828-19837.	1.9	2
2365	Nature of Beryllium, Magnesium, and Zinc Bonds in Carbeneâ< MX2 (M = Be, Mg, Zn; X = H, Br) Dimers Revealed by the IQA, ETS-NOCV and LED Methods. International Journal of Molecular Sciences, 2022, 23, 14668.	1.8	2
2366	Synthesis and Computational and X-ray Structure of 2, 3, 5-Triphenyl Tetrazolium, 5-Ethyl-5-phenylbarbituric Acid Salt. Crystals, 2022, 12, 1706.	1.0	7
2367	Reductive Decomposition Kinetics and Thermodynamics That Govern the Design of Fluorinated Alkoxyaluminate/Borate Salts for Mg-Ion and Ca-Ion Batteries. Journal of Physical Chemistry C, 2022, 126, 20773-20785.	1.5	5
2368	Development and Applications of the Density-Based Theory of Chemical Reactivity. Journal of Physical Chemistry Letters, 2022, 13, 11191-11200.	2.1	21
2369	Quantum mechanical study on complexation phenomenon of pillar[5]arene towards neutral dicyanobutane. Supramolecular Chemistry, 2021, 33, 634-646.	1.5	Ο

#	Article	IF	Citations
2370	Polymorphism and Mechanochromism in 2-Phenylbenzothiazole Cyclometalated Pt <sup>II</sup> Complexes with Chelating N <sup>â^§</sup> O Ligands. Inorganic Chemistry, 2022, 61, 20043-20056.	1.9	7
2371	Paramagnetic Semiconducting Se–Mn Clusters: A Mn <sub>3</sub> Se <sub>4</sub> -Stabilized Selenide Radical Intermediate and Its Aggregated Derivatives. Inorganic Chemistry, 2022, 61, 20433-20444.	1.9	1
2372	π-Extended Rubrenes via Dearomative Annulative π-Extension Reaction. Journal of the American Chemical Society, 2023, 145, 658-666.	6.6	6
2373	Mechanistic Investigation on Dearomative Spirocyclization of Arenes with α-Diazoamide under Boron Catalysis. ACS Catalysis, 2023, 13, 147-157.	5.5	3
2374	A Density Functional Theory Study on the Cobalt-Mediated Intramolecular Pauson–Khand Reaction of Enynes Containing a Vinyl Fluoride Moiety. Synthesis, 2023, 55, 1139-1149.	1.2	1
2375	Unveiling novel reactivity of P/Al frustrated Lewis pair: ring size-dependent activation of cyclic ethers/thioethers and CO2 insertion therein. Journal of Chemical Sciences, 2022, 134, .	0.7	4
2376	Dissecting Bonding Interactions in Cysteine Dimers. Molecules, 2022, 27, 8665.	1.7	1
2377	S–H···O Hydrogen Bond Can Win over O–H··S Hydrogen Bond: Gas-Phase Spectroscopy of 2-Fluorothiophenol···H <sub>2</sub> O Complex. Journal of Physical Chemistry A, 2022, 126, 9178-9189.	1.1	2
2378	Structures and Supramolecular Properties of Inclusion Complexes of Anthracene–Triptycene Nanocages with Fullerene Guests and Their Dynamic Motion as Molecular Gyroscopes. Chemistry - A European Journal, 0, , .	1.7	2
2379	Selenoxides as Excellent Chalcogen Bond Donors: Effect of Metal Coordination. Molecules, 2022, 27, 8837.	1.7	2
2380	Metal chelation ability of Protocatechuic acid anion with 210Po84; a theoretical insight. Computational and Theoretical Chemistry, 2023, 1220, 113996.	1.1	9
2381	Solution, Crystal and inâ€Silico Structures of the Organometallic Vitamin B12â€Derivative Acetylcobalamin and of its Novel Rhodiumâ€Analogue Acetylrhodibalamin. Helvetica Chimica Acta, 0, , .	1.0	0
2382	Thermally Controlled Exciplex Fluorescence in a Dynamic Homo[2]catenane. Journal of the American Chemical Society, 2022, 144, 23551-23559.	6.6	12
2383	<i>Inâ€Silico</i> Partial N <sub>2</sub> to NH <sub>3</sub> Conversion with a Light Atom Molecule. ChemPhysChem, 2023, 24, .	1.0	1
2384	X-ray Structures and Computational Studies of Two Bioactive 2-(Adamantane-1-carbonyl)-N-substituted Hydrazine-1-carbothioamides. Molecules, 2022, 27, 8425.	1.7	1
2385	Kinetically Stabilized Diarylpnictogenium Ions. ChemPlusChem, 2023, 88, .	1.3	1
2386	A Tetranuclear Ni(II)-Cubane Cluster Molecule Build by Four µ3-O-Methanolate (MeO) Ligands, Externally Cohesive by Four Unprecedented Bridging µ2-N7,O6-Acyclovirate (acv-H) Anions. Crystals, 2023, 13, 7.	1.0	1
2387	Uncovered Effects of thieno[2,3- <i>b</i> ]thiophene Substructure in a Tetrathienoacene Backbone: Reorganization Energy and Intermolecular Interaction. Chemistry of Materials, 2023, 35, 280-288.	3.2	6

#	Article	IF	CITATIONS
2389	Conformational preference analysis in C <sub>2</sub> H <sub>6</sub> using orbital forces and non-covalent interactions; comparison with related systems. Physical Chemistry Chemical Physics, 2023, 25, 4276-4283.	1.3	1
2390	H-Bonding leading to latent initiators for olefin metathesis polymerization. Faraday Discussions, 0, 244, 252-268.	1.6	4
2391	Room Temperature Fluoranthene Synthesis through Cationic Rh(I)/H <sub>8</sub> -BINAP-Catalyzed [2 + 2] Cycloaddition: Unexpected Acceleration due to Noncovalent Interactions. ACS Catalysis, 2023, 13, 1604-1613.	5.5	5
2392	Seâ< ï̃€ Chalcogen Bonding in 1,2,4-Selenodiazolium Tetraphenylborate Complexes. Symmetry, 2023, 15, 212.	1.1	7
2393	Mechanochemical Molecular Motion Using Noncovalent Interactions on Graphene and Its Application to Tailoring the Adsorption Energetics. , 2023, 5, 574-579.		4
2394	Decontamination of enoxacin containing aqueous phase through hydrophobic deep eutectic solvents: Solvent regeneration and quantum chemical insights. Journal of Molecular Liquids, 2023, 374, 121254.	2.3	4
2395	An insight into the non-covalent interactions in the solid state structures of dinuclear cobalt( <scp>ii</scp> ) complexes with N,O-donor ligands: application of the complexes in the fabrication of Schottky devices. CrystEngComm, 2023, 25, 1006-1017.	1.3	3
2396	Iodineâ€Catalyzed Claisenâ€Rearrangements of Allyl Aryl Ethers and Subsequent Iodocyclizations. Chemistry - an Asian Journal, 2023, 18, .	1.7	6
2397	Deciphering electronic and structural effects in Copper Corrole/Graphene Hybrids. Chemistry - A European Journal, 0, , .	1.7	0
2398	Unveiling the Mg( <scp>ii</scp> ) promoted [3+2] cycloaddition reaction of mesitonitrile oxide to Baylis–Hilman adduct from the molecular electron density theory perspective. New Journal of Chemistry, 2023, 47, 2495-2506.	1.4	1
2399	Halogen Bonding Channels for Magnetic Exchange in Cu(II) Complexes with 2,5â€Đi(methylthio)â€1,3,4â€ŧhiadiazole. Chemistry - an Asian Journal, 2023, 18, .	1.7	4
2400	Collective stabilization through n→ï€* and Pâ€¦ï€ phosphorous bonding with cooperative halogen and hydrogen bonding in POCl3-Nitrile dimers: Matrix isolation infrared spectroscopic and ab initio computational studies. Journal of Molecular Structure, 2023, 1278, 134916.	1.8	0
2401	Reliable Detection of Fluoroquinolones in Pharmaâ€effluents: Increasing Exposure in Environment Triggers Rise of Antimicrobial Resistance. ChemistrySelect, 2023, 8, .	0.7	0
2402	Helical coordination complex of Hg(ClO4)2 with bulky hydrazone derivative: A Möbius-like discrete metal chelate. Inorganic Chemistry Communication, 2023, 149, 110393.	1.8	1
2403	Experimental and theoretical study on photochromism of triphenylvinyl-naphthopyrans. Dyes and Pigments, 2023, 211, 111070.	2.0	2
2404	Synthesis of phenazone based carboxamide under thiourea reaction conditions. Molecular and crystal structure, Hirshfeld surface analysis and intermolecular interaction energies. Journal of Molecular Structure, 2023, 1278, 134948.	1.8	3
2405	Triphenylantimony(V) Complexes Based on o-Aminophenols with the Ambivalent N-Aryl Group. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2022, 48, 902-908.	0.3	1
2406	Ï€-Stacking Isomerism in Polycyclic Aromatic Hydrocarbons: The 2-Naphthalenethiol Dimer. Journal of Physical Chemistry Letters, 2023, 14, 207-213.	2.1	7

#	Article	IF	CITATIONS
2407	Ab Initio Metadynamics Simulations of Hexafluoroisopropanol Solvent Effects: Synergistic Role of Solvent Hâ€Bonding Networks and Solventâ€Solute Câ^H/ľ€ Interactions. Chemistry - A European Journal, 2023, 29, .	1.7	3
2408	Structural Factors That Determine the Activity of the Xenobiotic Reductase B Enzyme from Pseudomonas putida on Nitroaromatic Compounds. International Journal of Molecular Sciences, 2023, 24, 400.	1.8	0
2409	<i>In silico</i> capture and activation of methane with light atom molecules. Physical Chemistry Chemical Physics, 2023, 25, 5656-5662.	1.3	1
2410	Applications of the quantum theory of atoms in molecules and the interacting quantum atoms methods to the study of hydrogen bonds. , 2023, , 431-468.		1
2411	Understanding the mechanism and regio―and stereo selectivity of [3 + 2] cycloaddition reactions between substituted azomethine ylide and 3,3,3― <scp>trifluoro</scp> â€1â€nitropropâ€1â€ene, within the molecular electron density theory. Journal of Computational Chemistry, 0, , .	1.5	1
2412	Matere Bonds in Technetium Compounds: CSD Survey and Theoretical Considerations. Crystals, 2023, 13, 187.	1.0	6
2413	Role of Noncovalent Interactions in Inducing High Enantioselectivity in an Alcohol Reductive Deoxygenation Reaction Involving a Planar Carbocationic Intermediate. Journal of the American Chemical Society, 2023, 145, 2884-2900.	6.6	10
2414	Experimental and theoretical analysis for the structural, FT-IR, NLO, NBO and RDG properties of lindane using DFT technique. AIP Conference Proceedings, 2023, , .	0.3	2
2415	Remote Steric Control of the Tetrahedral Coordination Geometry around Heteroleptic Copper(I) Bis(Diimine) Complexes. Molecules, 2023, 28, 983.	1.7	1
2416	Exploring the Limits of Intramolecular London Dispersion Stabilization with Bulky Dispersion Energy Donors in Alkane Solution. Journal of the American Chemical Society, 2023, 145, 2093-2097.	6.6	9
2417	Extracting Quantitative Information at Quantum Mechanical Level from Noncovalent Interaction Index Analyses. Journal of Chemical Theory and Computation, 0, , .	2.3	1
2418	Stereospecific Oxycyanation of Alkenes with Sulfonyl Cyanide. Angewandte Chemie, 0, , .	1.6	0
2419	<b>TEtraQuinolines: A Missing Link in the Family of Porphyrinoid Macrocycles</b> . Journal of the American Chemical Society, 2023, 145, 2609-2618.	6.6	15
2420	Stereospecific Oxycyanation of Alkenes with Sulfonyl Cyanide. Angewandte Chemie - International Edition, 0, , .	7.2	2
2421	Mesomeric Betaines Based on Adamantylated 1,2,4â€Triazolo[4,3â€ <i>a</i> ]pyrimidinâ€5â€ones: Synthesis, Structure and Conversion into Anionic Nâ€Heterocyclic Carbenes. Chemistry - an Asian Journal, 2023, 18,	1.7	2
2422	Supramolecular Assemblies in Pyridine- and Pyrazole-Based Coordination Compounds of Co(II) and Ni(II): Characterization, Hirshfeld Analysis and Theoretical Studies. Crystals, 2023, 13, 203.	1.0	2
2423	Influence of non-covalent interactions on the coordination geometry of Ni( <scp>ii</scp> ) in Ni( <scp>ii</scp> )–M( <scp>ii</scp> ) complexes (M = Zn and Hg) with a salen-type N <sub>2</sub> O <sub>2</sub> Schiff base ligand and thiocyanate ion as the coligand. CrystEngComm, 2023, 25, 1393-1402.	1.3	1
2424	Quantum Chemical Studies on the Adsorption of Hexachlorobenzene, Decachlorobiphenyl, Benzene, and Biphenyl by BN-Doped Graphene and C-Doped Hexagonal Boron Nitride Modified with β-Cyclodextrin. Crystals, 2023, 13, 266.	1.0	1

#	Article	IF	CITATIONS
2425	Bringing Machineâ€Learning Enhanced Quantum Chemistry and Microwave Spectroscopy to Conformational Landscape Exploration: the Paradigmatic Case of 4â€Fluoroâ€Threonine. Chemistry - A European Journal, 2023, 29, .	1.7	8
2426	Regulation of ESIPT process based on aromaticity of cyanine dye molecules. Journal of Luminescence, 2023, 257, 119735.	1.5	6
2427	Nature of the dative Nitrogen-Coinage metal bond in molecular Motors. Evaluation of NHC-M pyrazine bond (MÂ=ÂCu, Ag, Au) from relativistic DFT. Inorganica Chimica Acta, 2023, 549, 121401.	1.2	0
2428	Computational approach to understanding the structures, properties, and supramolecular chemistry of pagoda[n]arenes. Journal of Molecular Structure, 2023, 1281, 135073.	1.8	1
2429	Density functional theory (DFT) computation of pristine and metal-doped MC59 (M = Au, Hf, Hg, Ir) fullerenes as nitrosourea drug delivery systems. Materials Science in Semiconductor Processing, 2023, 158, 107362.	1.9	20
2430	The importance of spodium bonds, H-bonds and π-stacking interactions in the solid state structures of four zinc complexes with tetradentate secondary diamine ligands. New Journal of Chemistry, 2023, 47, 9346-9363.	1.4	4
2431	Selective and efficient detection of Pb <sup>2+</sup> in aqueous solution by lanthanoid-organic frameworks bearing pyridine-3,4-dicarboxylic acid and glutaric acid. CrystEngComm, 2023, 25, 2418-2440.	1.3	2
2432	Visualization Analysis of Weak Interactions in Chemical Systems. , 2024, , 240-264.		10
2433	Metal-free catalytic conversion of CO <sub>2</sub> into methanol: local electrophilicity as a tunable property in the design and performance of aniline-derived aminoborane-based FLPs. Inorganic Chemistry Frontiers, 2023, 10, 2344-2358.	3.0	5
2434	Group-10 π-hole⋯d <sub><i>z</i><sup>2</sup></sub> [M <sup>II</sup> ] interactions: a theoretical study of model systems inspired by CSD structures. Dalton Transactions, 0, , .	1.6	2
2435	One-step synthesis of polycyclic thianthrenes from unfunctionalized aromatics by thia-APEX reactions. Organic Chemistry Frontiers, 2023, 10, 1880-1889.	2.3	2
2436	Covalent Triazine Framework C6N6 as an Electrochemical Sensor for Hydrogen-Containing Industrial Pollutants. A DFT Study. Nanomaterials, 2023, 13, 1121.	1.9	3
2437	Computational Study of Driving Forces in ATSP, PDIQ, and P53 Peptide Binding: Câ•O···Câ•O Tetrel Bonding Interactions at Work. Journal of Chemical Information and Modeling, 0, , .	2.5	0
2438	Theoretical evaluation of boron carbide nanotubes as non-enzymatic glucose sensors. Chemical Physics Letters, 2023, 823, 140510.	1.2	0
2439	Removal of highly concentrated methylene blue dye by cellulose nanofiber biocomposites. International Journal of Biological Macromolecules, 2023, 238, 124045.	3.6	7
2440	A combined experimental and theoretical study of covalent vs noncovalent dimer formation in vanadium(V) complexes with Schiff base ligands. Polyhedron, 2023, 235, 116335.	1.0	1
2441	Diamondoid as potential nonlinear optical material by superalkali doping: A first principles study. Diamond and Related Materials, 2023, 135, 109826.	1.8	9
2442	Mechanisms and origins of stereoselectivity involved in NHC-catalyzed [3Â+Â3] Annulation of 2-bromoenals and β-ketothioamides: A DFT study. Molecular Catalysis, 2023, 542, 113135.	1.0	0

#	Article	IF	CITATIONS
2443	Cooperativity effects in a new pterostilbene/phenanthroline cocrystal. Journal of Molecular Structure, 2023, 1282, 135227.	1.8	0
2444	Reversible hydrogen storage on multiple Ti-doped B12C6N6 nanocage. Journal of Energy Storage, 2023, 62, 106910.	3.9	3
2445	Fluorescent properties based on ESIPT and TICT of novel acylhydrazone-based probe and its sensing mechanism for Al3+: A TD-DFT investigation. Journal of Molecular Liquids, 2023, 379, 121639.	2.3	1
2446	Combined experimental and theoretical studies of bis-chalcone: Estimation of non-covalent interactions. Journal of Molecular Structure, 2023, 1282, 135189.	1.8	2
2447	Intriguing π-interactions involving aromatic neutrals, aromatic cations and semiconducting behavior in a pyridinium-carboxylate salt. Journal of Molecular Structure, 2023, 1284, 135326.	1.8	5
2448	Fluorescent deactivation behaviors based on ESIPT and TICT of novel double target fluorescent probe and its sensing mechanism for Al3+/Mg2+: A TD-DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2023, 297, 122718.	2.0	1
2449	Insight into the role of pseudo-halides as multiple hydrogen bond acceptors in the formation of supramolecular 1D assembly of di and trinuclear zinc complexes. Inorganica Chimica Acta, 2023, 553, 121516.	1.2	2
2450	Design, synthesis, and computational studies of novel imidazo[1,2-a]pyrimidine derivatives as potential dual inhibitors of hACE2 and spike protein for blocking SARS-CoV-2 cell entry. Journal of Molecular Structure, 2023, 1285, 135525.	1.8	3
2451	A novel use of an oxime molecule as supramolecular tecton. Synthesis of a Pt (II) 2D network. Journal of Molecular Structure, 2023, 1285, 135485.	1.8	0
2452	Linear and Bent Cp* <sub>2</sub> Si: Reversible Phase Transition of a Key Molecule. Angewandte Chemie - International Edition, 2023, 62, .	7.2	0
2453	Removal of methylene blue by using sodium alginate-based hydrogel; validation of experimental findings via DFT calculations. Journal of Molecular Graphics and Modelling, 2023, 122, 108468.	1.3	12
2454	Different competition mechanism between ESPT and TICT process regulated by protic and aprotic solvent in DHP. Journal of Molecular Liquids, 2023, 375, 121278.	2.3	3
2455	Antioxidant activity and enzymatic of lichen substances: A study based on cyclic voltammetry and theoretical. Chemico-Biological Interactions, 2023, 372, 110357.	1.7	5
2456	Revealing the supramolecular interactions of the bis(azopyrenyl) dibenzo-18-crown-6-ether system. Journal of Molecular Liquids, 2023, 374, 121298.	2.3	1
2457	Insights into the CO <sub>2</sub> Capture Capacity of Covalent Organic Frameworks. ChemPhysChem, 2023, 24, .	1.0	2
2458	A Comparison of Non-Covalent Interactions in the Crystal Structures of two σ-Alkane Complexes of Rh Exhibiting Contrasting Stabilities in the Solid State Faraday Discussions, 0, , .	1.6	1
2459	Boat and Chair Shaped Hexahalogen Synthons. Chemistry - an Asian Journal, 2023, 18, .	1.7	3
2460	Comparative study of the efficiency of silicon carbide, boron nitride and carbon nanotube to deliver cancerous drug, azacitidine: A DFT study. Computers in Biology and Medicine, 2023, 154, 106593.	3.9	7

IF CITATIONS

2461	Structural and electronic properties of the Metal-Organic Frameworks Mâ^'URJCâ^'1 (MÂ=ÂCu, Fe, Co or) Tj ETQqC 116324.	0 0 rgBT 1.0	/Overlock 1 3
2462	Metallic–Organic Cages (MOCs) with Heterometallic Character: Flexibility-Enhancing MOFs. Catalysts, 2023, 13, 317.	1.6	Ο
2463	Structural, Spectral, Molecular Docking, and Molecular Dynamics Simulations of Phenylthiophene-2-Carboxylate Compounds as Potential Anticancer Agents. Polycyclic Aromatic Compounds, 2024, 44, 238-260.	1.4	20
2464	Experimental and Theoretical Study of Tetrel Bonding and Noncovalent Interactions in Hemidirected Lead(II) Phosphorodithioates: An Implication on Crystal Engineering. Crystal Growth and Design, 2023, 23, 2138-2154.	1.4	2
2465	Distal Mutations in the β-Clamp of DNA Polymerase III* Disrupt DNA Orientation and Affect Exonuclease Activity. Journal of the American Chemical Society, 2023, 145, 3478-3490.	6.6	2
2466	Discrete Singular Metallophilic Interaction in Stable Large 12-Membered Binuclear Silver and Gold Metallamacrocycles of Amido-Functionalized Imidazole and 1,2,4-Triazole-Derived N-Heterocyclic Carbenes. ACS Omega, 2023, 8, 6439-6454.	1.6	0
2467	Computational Evidence of the Incipient Oxocarbenium Ion as a "Hidden Intermediate―During the Cyclization of Hydroxyenol Ether into Spiroketal Under Mild Acidic Condition. Chemistry - A European Journal, 0, , .	1.7	0
2468	Reactivity of a model of B3P3-doped nanographene with up to three CO2 molecules. Scientific Reports, 2023, 13, .	1.6	4
2469	Theoretical Study on the Origin of Abnormal Regioselectivity in Ring-Opening Reaction of Hexafluoropropylene Oxide. Molecules, 2023, 28, 1669.	1.7	0
2470	Conformational analysis of cyclohexyl hydroperoxide by rotational spectroscopy. Journal of Molecular Spectroscopy, 2023, 392, 111758.	0.4	2
2471	Tuning charge carrier dynamics through spacer cation functionalization in layered halide perovskites: an <i>ab initio</i> quantum dynamics study. Journal of Materials Chemistry C, 2023, 11, 3521-3532.	2.7	0
2472	The impact of SARS-CoV-2 3CL protease mutations on nirmatrelvir inhibitory efficiency. Computational insights into potential resistance mechanisms. Chemical Science, 2023, 14, 2686-2697.	3.7	6
2473	Geminal Charge-Assisted Tetrel Bonds in Bis-Pyridinium Methylene Salts. Crystal Growth and Design, 2023, 23, 1898-1902.	1.4	2
2474	Square Planar Pt(II) Ion as Electron Donor in Pnictogen Bonding Interactions. Inorganics, 2023, 11, 80.	1.2	2
2475	Mechanistic insight into the ligand-controlled regioselective hydrocarboxylation of aryl olefins with palladium catalyst: A computational study. Journal of Organometallic Chemistry, 2023, 989, 122645.	0.8	0
2476	In Silico Investigation of the Molecular Mechanism of PARP1 Inhibition for the Treatment of BRCA-Deficient Cancers. Molecules, 2023, 28, 1829.	1.7	1
2477	Mechanism of Co( <scp>iii</scp> )-catalyzed annulation of <i>N</i> -chlorobenzamide with styrene and origin of cyclopentadienyl ligand-controlled enantioselectivity. Organic Chemistry Frontiers, 2023, 10, 1643-1650.	2.3	2
2478	Self-Sorting of Transient Polymer Networks by the Selective Formation of Heteroleptic Metal–Ligand Complexes. Macromolecules, 2023, 56, 1390-1401.	2.2	4

#

ARTICLE

CITA	TION	DEDODT
LIIA	IION.	Report

#	Article	IF	CITATIONS
2479	Charging and Electric Field Effects on Hydrogen Molecules Physisorbed on Graphene. Journal of Physical Chemistry C, 2023, 127, 4326-4333.	1.5	4
2480	Detailed analysis of distorted retinal and its interaction with surrounding residues in the K intermediate of bacteriorhodopsin. Communications Biology, 2023, 6, .	2.0	2
2481	Halogen Bondâ€Involving Supramolecular Assembly Utilizing Carbon as a Nucleophilic Partner of Iâ‹â‹â‹C Nonâ€covalent Interaction. Chemistry - an Asian Journal, 2023, 18, .	1.7	5
2482	Chemical sensing ability of aminated graphdiyne (GDY-NH2) toward highly toxic organic volatile pollutants. Computational and Theoretical Chemistry, 2023, 1222, 114079.	1.1	3
2483	NHCâ€Stabilised Parent Tripentelyltrielanes. Chemistry - A European Journal, 2023, 29, .	1.7	1
2484	Metal ion-decorated hexasilaprismane and its derivative as a molecular container for the separation of CO <sub>2</sub> from flue gas molecules: a computational study. Dalton Transactions, 2023, 52, 4336-4348.	1.6	0
2485	Solid State. Theoretical Chemistry and Computational Modelling, 2023, , 253-297.	0.2	0
2486	Weak Interactions. Theoretical Chemistry and Computational Modelling, 2023, , 175-218.	0.2	0
2487	DFT calculations predict that inverted geometries at carbon can be stabilized within multi-component co-crystals. Theoretical Chemistry Accounts, 2023, 142, .	0.5	0
2488	Unconventional Dual Donor-Acceptor Topologies of Aromatic Rings in Amine-Based Polymeric Tetrahedral Zn(II) Compounds Involving Unusual Non-Covalent Contacts: Antiproliferative Evaluation and Theoretical Studies. Crystals, 2023, 13, 382.	1.0	2
2489	Rational Coformer Selection in the Development of 6-Propyl-2-thiouracil Pharmaceutical Cocrystals. Pharmaceuticals, 2023, 16, 370.	1.7	0
2490	The Ultrashort Spike–Ring Interaction in Substituted Iron Maiden Molecules. Molecules, 2023, 28, 2244.	1.7	1
2491	Synthesis of 4-Amino-N-[2 (diethylamino)Ethyl]Benzamide Tetraphenylborate Ion-Associate Complex: Characterization, Antibacterial and Computational Study. Molecules, 2023, 28, 2256.	1.7	5
2492	Synthesis of a Ï€â€Extended Double [9]Helicene. Angewandte Chemie - International Edition, 2023, 62, .	7.2	11
2493	Synthesis of a Ï€â€Extended Double [9]Helicene. Angewandte Chemie, 2023, 135, .	1.6	0
2494	Lineares und gewickeltes Cp* <sub>2</sub> Si: Reversibler Phasendurchgang eines Schlüsselmoleküls. Angewandte Chemie, 2023, 135, .	1.6	0
2495	Synthesis, X-ray characterization and DFT calculations of a series of 3-substituted 4,5-dichloroisothiazoles. CrystEngComm, 2023, 25, 1976-1985.	1.3	0
2496	Substituent Effects in Tetrel Bonds Involving Aromatic Silane Derivatives: An ab initio Study. Molecules, 2023, 28, 2385.	1.7	0

#	Article	IF	CITATIONS
2497	Experimental and computational studies of tautomerism pyridine carbonyl thiosemicarbazide derivatives. Structural Chemistry, 0, , .	1.0	2
2498	Cocrystallization of Antifungal Compounds Mediated by Halogen Bonding. Crystal Growth and Design, 2023, 23, 2932-2940.	1.4	6
2499	Comprehensive Mechanistic Scenario for the Cu-Mediated Asymmetric Propargylic Sulfonylation Forging Tertiary Carbon Stereocenters. Journal of the American Chemical Society, 2023, 145, 6442-6452.	6.6	11
2500	Gas phase electronic spectra of xylene-water aggregates. Journal of Molecular Spectroscopy, 2023, 393, 111761.	0.4	0
2502	An investigation of Solidâ€ <b>s</b> tate Emission of Halogenated Diphenyl Phosphanyl Anthracenes. Advanced Optical Materials, 0, , 2202753.	3.6	1
2503	Double Hook Perylene Diimide as a New Receptor for PAHs: An Experimental and Theoretical Study. ChemPhysChem, 0, , .	1.0	0
2504	Structure and stability of the <scp>sH</scp> binary hydrate cavity and <scp>hostâ€guest</scp> versus <scp>guestâ€guest</scp> interactions therein: A <scp>DFT</scp> approach. Journal of Computational Chemistry, 2023, 44, 1446-1453.	1.5	0
2505	A Comprehensive Ab Initio Study of Halogenated A···U and C···C Base Pair Geometries and Energies. International Journal of Molecular Sciences, 2023, 24, 5530.	1.8	2
2506	A Theoretical Analysis of Interaction Energies and Intermolecular Interactions between Amphotericin B and Potential Bioconjugates Used in the Modification of Nanocarriers for Drug Delivery. Molecules, 2023, 28, 2674.	1.7	3
2507	The study of the PES and the reaction mechanism between ketene and Lithium Carbenoids and the formation of cyclopropanone. Theoretical Chemistry Accounts, 2023, 142, .	0.5	0
2508	Cooperativity and intermolecular hydrogen bonding in donorâ€acceptor complexes of phenol and polyhydroxybenzenes. Journal of Physical Organic Chemistry, 2023, 36, .	0.9	1
2509	Cooperative Ternary Assemblies Involving Anion–Ĩ€/Ĩ€â€"Ĩ€/Anion–Ĩ€ Assemblies and Unconventional Clâ< Cl Interactions in Cu(II) Coordination Compounds: Experimental and Theoretical Studies. Crystals, 2023, 13, 517.	1.0	3
2510	Selective Detection of Copper Ions and Biological Activities of Isoniazid Schiff Bases. ChemistrySelect, 2023, 8, .	0.7	1
2511	Understanding and Describing London Dispersion Effects in ÂTransition-Metal-Catalyzed C–H Activations. Synlett, 2023, 34, 1098-1112.	1.0	1
2512	Molecular Assembly of Rhodanine with Torusâ€5haped Cyclodextrins and Their Innovative Applications by Physicochemical Contrivance Simultaneously Optimized by Computational Study. ChemistrySelect, 2023, 8, .	0.7	0
2513	Screening Physical Solvents for Methyl Mercaptan Absorption Using Quantum Chemical Calculation Coupled with Experiments. ACS Omega, 2023, 8, 11790-11800.	1.6	0
2514	Exploration of Diverse Interactions of <scp>l</scp> -Methionine in Aqueous Ionic Liquid Solutions: Insights from Experimental and Theoretical Studies. ACS Omega, 2023, 8, 12098-12123.	1.6	3
2515	Hydrogen bonding guest-water interactions in pinacolone, tert-butyl amine, and tert-butylmethyl ether: a theoretical study on energetics, structure, and topological +. Journal of Molecular Modeling, 2023, 29, .	0.8	1

#	Article	IF	CITATIONS
2516	Complexation behaviour of piceatannol ligand with Ti(IV) and Zr(IV) metal ions: a combined DFT and deep learning investigation. Structural Chemistry, 2023, 34, 2139-2152.	1.0	3
2517	Divergent Rh Catalysis: Asymmetric Dearomatization Versus C–H Activation Initiated by C–C Activation. ACS Catalysis, 2023, 13, 4873-4881.	5.5	6
2518	Propane Oxidative Dehydrogenation on Nanosized Boron Carbide: Effect of Boron Content and Its Oxidation Implicated by DFT Calculations. Journal of Physical Chemistry C, 2023, 127, 6280-6293.	1.5	0
2519	Quantitative analysis of the interplay of hydrogen bonds in M(II)-hexaaqua complexes with HMTA [M(II)Â=ÂCo(II), Mg(II); HMTAÂ=Ahexamethylenetetramine]. Journal of Molecular Structure, 2023, 1284, 135448.	1.8	7
2520	Principles of Catalysis. Engineering Materials, 2023, , 95-113.	0.3	0
2521	Lithium-Mediated Mechanochemical Cyclodehydrogenation. Journal of the American Chemical Society, 2023, 145, 8163-8175.	6.6	5
2522	Effect of Substituents on the Intramolecular n→ï€* Interaction in 3-[2-(Dimethylamino) phenyl] propanal: A Computational Study. Journal of Physical Chemistry A, 2023, 127, 3339-3346.	1.1	2
2523	Tetrel bonds involving CF3 group participate in protein-drug recognition: A combined crystallographic and computational study Physical Chemistry Chemical Physics, 0, , .	1.3	0
2524	Two triplet emitting states in one emitter: Near-infrared dual-phosphorescent Au <sub>20</sub> nanocluster. Science Advances, 2023, 9, .	4.7	22
2525	Insights on adsorption properties of a DNA base, guanine on nano metal cages (Ag24/Au24/Cu24): DFT, SERS, NCI and solvent effects. Journal of Molecular Structure, 2023, 1285, 135541.	1.8	4
2526	Organocatalytic Enantioselective Vinylcyclopropane yclopentene (VCP P) Rearrangement. Angewandte Chemie - International Edition, 2023, 62, .	7.2	5
2527	Organocatalytic Enantioselective Vinylcyclopropane yclopentene (VCP P) Rearrangement. Angewandte Chemie, 0, , .	1.6	0
2528	Encapsulation of Astatide by a water cage. Physical Chemistry Chemical Physics, 0, , .	1.3	1
2529	Aromaticity of Cope and Claisen rearrangements. Theoretical Chemistry Accounts, 2023, 142, .	0.5	3
2530	Clay-supported acidic ionic liquid as an efficient catalyst for conversion of carbohydrates to 5-hydroxymethylfurfural. Journal of Molecular Liquids, 2023, 382, 121847.	2.3	14
2531	Effect of confinement and external mechanical force on the cleavage of the bond in a diatomic molecule. Molecular Physics, 0, , .	0.8	0
2532	Sulfur–arene interactions: the Sâ<-ï€ and S–Hâ<-ï€ interactions in the dimers of benzofuranâ< sulfur dioxide and benzofuranâ< hydrogen sulfide. Physical Chemistry Chemical Physics, 2023, 25, 12174-12181.	1.3	2
2533	Engineering Host–Guest Interactions in Organic Framework Materials for Drug Delivery. Helvetica Chimica Acta, 2023, 106, .	1.0	1

#	Article	IF	CITATIONS
2534	Pnictogen Bonding Enabled Photosynthesis of Chiral Selenium-Containing Pyridines from Pyridylphosphonium Salts. Fundamental Research, 2023, , .	1.6	2
2535	Unveiling the exclusive stereo and site selectivity in [3+2] cycloaddition reactions of a tricyclic strained alkene with nitrile oxides from the molecular electron density theory perspective. Chemistry of Heterocyclic Compounds, 0, , .	0.6	2
2536	Crystal Structures of 3,3′,5,5′-Tetrabromo-4,4′-bipyridine and Co(II) Coordination Polymer Based Thereon Crystals, 2023, 13, 704.	1.0	1
2537	Regiumâ~ï̃€ Bonds Involving Nucleobases: Theoretical Study and Biological Implications. Inorganic Chemistry, 2023, 62, 6740-6750.	1.9	4
2551	Beyond QTAIM: NCI Indexes as a Tool to Reveal Intermolecular Bonds in Molecular Aggregates. , 2017, , 222-257.		0
2558	Insights into the coordination chemistry of antineoplastic doxorubicin with 3d-transition metal ions Zn2+, Cu2+, and VO2+: a study using well-calibrated thermodynamic cycles and chemical interaction quantum chemistry models. Journal of Computer-Aided Molecular Design, 2023, 37, 279-299.	1.3	0
2584	Unified Classification of Non-Covalent Bonds Formed by Main Group Elements: A Bridge to Chemical Bonding. Physical Chemistry Chemical Physics, 0, , .	1.3	0
2586	Modification of QuinoxP*-Type Bisphosphine Ligands for High-Performance Asymmetric Boryl Substitution of Racemic Allyl Electrophiles. Springer Theses, 2023, , 19-112.	0.0	0
2589	Computational Investigation on Copper(I)-Catalyzed Enantioselective Radical Borylation of Benzyl Halides. Springer Theses, 2023, , 213-223.	0.0	0
2590	Factors driving the Ni/Cu cooperative asymmetric propargylation of aldimine esters. Chemical Communications, 2023, 59, 6521-6524.	2.2	2
2616	The use of molecular electronic structure methods to investigate mechanically interlocked molecules. Physical Chemistry Chemical Physics, 2023, 25, 19409-19421.	1.3	3
2660	Halogen bonding in chloroiodates(III). CrystEngComm, 0, , .	1.3	0
2678	Enzymatic reversion of Pt( <scp>ii</scp> ) nucleophilicity through charge dumping: the case of Pt(CN) <sub>4</sub> <sup>2â^'</sup> . Chemical Communications, 0, , .	2.2	0
2691	Exploring the influence of graphene on antiaromaticity of pentalene. Physical Chemistry Chemical Physics, 2023, 25, 26986-26990.	1.3	0
2732	Half-substituted fluorocycloparaphenylenes with high symmetry: Synthesis, properties and derivatization to densely substituted carbon nanorings. Chemical Communications, 0, , .	2.2	1