

Antonio Frontera

List of Publications by Year in descending order

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802
papers

27,203
citations

9264

74
h-index

17105

122
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836
all docs

836
docs citations

836
times ranked

12736
citing authors

#	ARTICLE	IF	CITATIONS
1	Favipiravir: insight into the crystal structure, Hirshfeld surface analysis and computational study. <i>Journal of the Iranian Chemical Society</i> , 2022, 19, 85-94.	2.2	26
2	Phenanthroline-based Ni(II) coordination compounds involving unconventional discrete fumarate-water-nitrate clusters and energetically significant cooperative ternary π -stacked assemblies: Antiproliferative evaluation and theoretical studies. <i>Journal of Molecular Structure</i> , 2022, 1248, 131424.	3.6	10
3	Lead(II) supramolecular structures formed through a cooperative influence of the hydrazinecarbothioamide derived and ancillary ligands. <i>CrystEngComm</i> , 2022, 24, 368-378.	2.6	7
4	Metal Centers as Nucleophiles: Oxymoron of Halogen Bonding Involving Crystal Engineering. <i>Chemistry - A European Journal</i> , 2022, 28, .	3.3	41
5	Seâ€¦â€¦â€¦O/S and Sâ€¦â€¦â€¦O Chalcogen Bonds in Small Molecules and Proteins: A Combined CSD and PDB Study. <i>ChemBioChem</i> , 2022, 23, e202100498.	2.6	27
6	A comparative study of noncovalent interactions in various Ni-compounds containing nitrogen heteroaromatic ligands and pseudohalides: A combined experimental and theoretical studies. <i>Inorganica Chimica Acta</i> , 2022, 531, 120702.	2.4	0
7	Energetic features of antiparallel stacking and hydrogen bonding interactions in two coordination complexes bearing 1,10-phenanthroline-2,9-dicarboxylic acid. <i>Journal of Molecular Structure</i> , 2022, 1251, 131963.	3.6	3
8	An insight into triel bonds in π -diarylphosphorodithioates of thallium(I): experimental and theoretical investigations. <i>New Journal of Chemistry</i> , 2022, 46, 832-843.	2.8	7
9	Synthesis, structural topologies and anticancer evaluation of phenanthroline-based 2,6-pyridinedicarboxylato Cu(II) and Ni(II) compounds. <i>Polyhedron</i> , 2022, 213, 115632.	2.2	6
10	Spodium bonds and metal-halogen-halogen-metal interactions in propagation of monomeric units to dimeric or polymeric architectures. <i>Journal of Molecular Structure</i> , 2022, 1252, 132144.	3.6	8
11	Solvothermal synthesis and crystal structures of two Holmium(III)-5-Hydroxyisophthalate entangled coordination polymers and theoretical studies on the importance of π -stacking interactions. <i>Journal of Molecular Structure</i> , 2022, 1254, 132329.	3.6	10
12	Multicomponent Solids of DL-2-Hydroxy-2-phenylacetic Acid and Pyridinecarboxamides. <i>Crystals</i> , 2022, 12, 142.	2.2	4
13	Frontispiece: Metal Centers as Nucleophiles: Oxymoron of Halogen Bonding Involving Crystal Engineering. <i>Chemistry - A European Journal</i> , 2022, 28, .	3.3	5
14	Host-guest complexes vs. supramolecular polymers in chalcogen bonding receptors: an experimental and theoretical study. <i>Dalton Transactions</i> , 2022, 51, 1325-1332.	3.3	6
15	Large interaction energy for the homodimer and the heterodimer extracted from the supramolecular chain of a bent trinuclear zinc(II) complex with a reduced Schiff base ligand. <i>New Journal of Chemistry</i> , 2022, 46, 1845-1856.	2.8	2
16	Aza-Crown-Based Macrocyclic Probe Design for PET-off Multi-Cu ²⁺ Responsive and CHEF-on Multi-Zn ²⁺ Sensor: Application in Biological Cell Imaging and Theoretical Studies. <i>Inorganic Chemistry</i> , 2022, 61, 1982-1996.	4.0	5
17	Oxalic Acid, a Versatile Coformer for Multicomponent Forms with 9-Ethyladenine. <i>Crystals</i> , 2022, 12, 89.	2.2	3
18	Syntheses, crystal structures and supramolecular assemblies of two Cu(II) complexes based on a new heterocyclic ligand: insights into π -H \cdot Cl and π - π interactions. <i>CrystEngComm</i> , 2022, 24, 1598-1611.	2.6	17

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19	Anion-catalysis Enabled by the Mechanical Bond**. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	20
20	Topochemical [2 + 2] Cycloaddition in a Two-Dimensional Metal-Organic Framework via SCSC Transformation Impacts Halogen-Halogen Interactions. <i>Inorganic Chemistry</i> , 2022, 61, 3029-3032.	4.0	10
21	Insight into charge transportation in cadmium based semiconducting organic-inorganic hybrid materials and their application in the fabrication of photosensitive Schottky devices. <i>Dalton Transactions</i> , 2022, 51, 5721-5734.	3.3	10
22	Enhancing chalcogen bonding by metal coordination. <i>Dalton Transactions</i> , 2022, , .	3.3	9
23	Metallophilic interactions in silver(<i>scpi</i>) dicyanoaurate complexes. <i>Dalton Transactions</i> , 2022, , .	3.3	1
24	Do 2-coordinate iodine(<i>scpi</i>) and silver(<i>scpi</i>) complexes form nucleophilic iodonium interactions (NIs) in solution?. <i>Chemical Communications</i> , 2022, 58, 4977-4980.	4.1	9
25	Chameleonic metal-bound isocyanides: a π -donating Cu ^I -center imparts nucleophilicity to the isocyanide carbon toward halogen bonding. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 1655-1665.	6.0	13
26	Structural topologies involving energetically significant antiparallel π -stacking and unconventional N(nitrile)- π (fumarate) contacts in dinuclear Zn(<i>scpii</i>) and polymeric Mn(<i>scpii</i>) compounds: antiproliferative evaluation and theoretical studies. <i>New Journal of Chemistry</i> , 2022, 46, 5296-5311.	2.8	7
27	Synthesis, spectroscopic findings and crystal engineering of Pb(<i>scpii</i>)-Salen coordination polymers, and supramolecular architectures engineered by f -hole/sodium/tetrel bonds: a combined experimental and theoretical investigation. <i>RSC Advances</i> , 2022, 12, 6352-6363.	3.6	25
28	Iodine(<i>scpi</i>) complexes incorporating sterically bulky 2-substituted pyridines. <i>RSC Advances</i> , 2022, 12, 8674-8682.	3.6	6
29	Solvent-driven structural topologies in phenanthroline-based co-crystals of Zn(<i>scpii</i>) involving fascinating infinite chair-like $\{[(bzH)_4Cl_2]^{2+}\}_n$ assemblies and unconventional layered infinite $\{bz-H_2O-Cl\}_n$ anion-water clusters: antiproliferative evaluation and theoretical studies. <i>New Journal of Chemistry</i> , 2022, 46, 5638-5652.	2.8	4
30	Anion-Responsive Fluorescent Supramolecular Gels. <i>Molecules</i> , 2022, 27, 1257.	3.8	10
31	Field-induced single-molecule magnet behaviour in a series of dinuclear cobalt(III,II) complexes. <i>Polyhedron</i> , 2022, 220, 115802.	2.2	5
32	Substituent Effects in π -Hole Regium Bonding Interactions Between Au(<i>ip</i>)- π (Py) ₂ Complexes and Lewis Bases: An <i>ab initio</i> Study. <i>ChemPhysChem</i> , 2022, , .	2.1	6
33	Direct conversion of white phosphorus to versatile phosphorus transfer reagents via oxidative oxidation. <i>Nature Chemistry</i> , 2022, 14, 384-391.	13.6	31
34	Anion- π stacks of Lindqvist superoctahedra [Mo ₆ O ₁₉] ²⁻ supported by caffeinium and theophyllinium cations. <i>Inorganica Chimica Acta</i> , 2022, 537, 120945.	2.4	2
35	Polymorphism in the 1/1 Pterostilbene/Picolinic Acid Cocrystal. <i>Crystal Growth and Design</i> , 2022, 22, 590-597.	3.0	10
36	Inorganic-organic $\{d_z^2\text{-}M\text{II}S_4\}$ -hole stacking in reverse sandwich structures: the case of cocrystals of group 10 metal dithiocarbamates with electron-deficient arenes. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 2869-2879.	6.0	9

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37	Zwitterionic iodonium species afford halogen bond-based porous organic frameworks. <i>Chemical Science</i> , 2022, 13, 5650-5658.	7.4	16
38	Metal Coordination Enhances Chalcogen Bonds: CSD Survey and Theoretical Calculations. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4188.	4.1	13
39	Supramolecular aggregation of lead(II) perchlorate and a thiosemicarbazide derivative linked by a myriad of non-covalent interactions. <i>Inorganica Chimica Acta</i> , 2022, 538, 120974.	2.4	4
40	Investigation of solid state architectures in tetrazolyl tryptophol stabilized by crucial aromatic interactions and hydrogen bonding: Experimental and theoretical analysis. <i>Journal of Molecular Structure</i> , 2022, 1262, 133079.	3.6	6
41	Role of Redox-Inactive Metal Ions in Modulating the Reduction Potential of Uranyl Schiff Base Complexes: Detailed Experimental and Theoretical Studies. <i>Inorganic Chemistry</i> , 2022, 61, 7130-7142.	4.0	6
42	On the energetic stability of halogen bonds involving metals: implications in crystal engineering. <i>CrystEngComm</i> , 2022, 24, 4440-4446.	2.6	15
43	On metal coordination of neutral open-shell P-ligands focusing on phosphanoxylys, their electron residence and reactivity. <i>Chemical Communications</i> , 2022, 58, 6270-6279.	4.1	3
44	Insight into non-covalent interactions in a [Cu(N ₃) ₄] ²⁺ bridged hetero-pentanuclear copper(II)/sodium complex with special emphasis on the strong CH⋯N[Cu(N ₃) ₄] interactions. <i>New Journal of Chemistry</i> , 2022, 46, 11286-11295.	2.8	7
45	Expanding the toolbox of the coinage bond: adducts involving new gold(III) derivatives and bioactive molecules. <i>CrystEngComm</i> , 2022, 24, 3846-3851.	2.6	8
46	Estimation of the ability of the π-system of pseudohalides (azide and thiocyanate) to participate in CH⋯π interactions in cyclic hetero-tetranuclear cobalt(III)/sodium and linear trinuclear mixed valence cobalt(III/II/III) complexes. <i>Polyhedron</i> , 2022, 222, 115862.	2.2	4
47	Supramolecular Assemblies Based on π-hole Interactions. , 2022, , 203-241.		1
48	Hydrogen and halogen bond synergy in the self-assembly of 3,5-dihalo-tyrosines: structural and theoretical insights. <i>CrystEngComm</i> , 2022, 24, 7255-7260.	2.6	1
49	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. <i>Polyhedron</i> , 2022, 223, 115910.	2.2	5
50	Exploration of supramolecular and theoretical aspects of two new Cu(II) complexes: On the importance of lone pair⋯π(chelate ring) and π⋯π(chelate ring) interactions. <i>Journal of Molecular Structure</i> , 2022, 1265, 133358.	3.6	5
51	Towards Anion Recognition and Precipitation with Water-Soluble 1,2,4-Selenodiazolium Salts: Combined Structural and Theoretical Study. <i>International Journal of Molecular Sciences</i> , 2022, 23, 6372.	4.1	16
52	Noncovalent Interactions Involving Group 6%in Biological Systems: The Case of Molybdopterin and Tungstopterin Cofactors. <i>Chemistry - A European Journal</i> , 2022, 28, .	3.3	21
53	Revision of the Crystal Structure of the Orthorhombic Polymorph of Oxyma: On the Importance of π⋯π-Hole Interactions and Their Interplay with H⋯Bonds. <i>Crystals</i> , 2022, 12, 823.	2.2	1
54	Terephthalato and succinato bridged Mn(II) and Zn(II) coordination polymers involving structure-guiding H-bonded tetrameric assemblies: Antiproliferative evaluation and theoretical studies. <i>Polyhedron</i> , 2022, 224, 115982.	2.2	3

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55	Antiparallel π - π and $C\equiv N\cdots H\cdots C$ contacts in a novel Zn(II) coordination solid involving π -hole tetrel bonding interactions: A combined experimental and theoretical study, Hirshfeld surface analysis, molecular docking and potential drug property. <i>Journal of Molecular Structure</i> , 2022, 1268, 133686.	3.6	4
56	Synthesis, characterization and self assembly of dinuclear zinc Schiff base complexes: A combined experimental and theoretical study. <i>Polyhedron</i> , 2022, 225, 116044.	2.2	5
57	DFT study on CH_3O , CH_3SCN and $S\cdots N$ interaction energies in three dinuclear mixed valence cobalt(III/II) complexes with secondary diamine ligands having inner N_2O_2 and outer O_4 compartments. <i>Polyhedron</i> , 2022, , 116039.	2.2	1
58	Supramolecular assemblies involving unconventional non-covalent contacts in pyrazole-based coordination compounds of Co(II) and Cu(II) pyridinedicarboxylates: Antiproliferative evaluation and theoretical studies. <i>Polyhedron</i> , 2022, 224, 116025.	2.2	2
59	Magnetically separable nanocatalyst (IL@CuFe ₂ O ₄ -L-Tyr-TiO ₂ /TiTCIL): Preparation, characterization and its applications in 1,2,3-triazole synthesis and in photodegradation of MB. <i>Journal of Molecular Structure</i> , 2021, 1224, 129029.	3.6	14
60	Two new hydrogen-bonded supramolecular dioxo-molybdenum(VI) complexes based on acetyl-hydrazone ligands: Synthesis, crystal structure and DFT studies. <i>Journal of Molecular Structure</i> , 2021, 1226, 129346.	3.6	10
61	Synthesis, X-ray characterization, Hirshfeld surface analysis and DFT calculations on tetrazolyl-phenol derivatives: H-bonds vs $C\equiv N\cdots N$ interactions. <i>Journal of Molecular Structure</i> , 2021, 1227, 129425.	3.6	9
62	An insight into the role of supramolecular interactions to stabilize the solid state structure of an octahedral nickel(II) diamine complex. <i>Inorganica Chimica Acta</i> , 2021, 515, 120023.	2.4	7
63	Energetically significant nitrile \cdots nitrile and unconventional $C\equiv N\cdots N$ interactions in pyridine based Ni(II) and Zn(II) coordination compounds: Antiproliferative evaluation and theoretical studies. <i>Journal of Molecular Structure</i> , 2021, 1223, 129246.	3.6	13
64	Bifurcated $\frac{1}{4}$ \cdots (N,O) Halogen Bonding: The Case of (Nitrosoguanidinate)Ni ^{II} Cocrystals with Iodine(I)-Based π -Hole Donors. <i>Crystal Growth and Design</i> , 2021, 21, 588-596.	3.0	24
65	Semiconducting properties of pyridyl appended linear dicarboxylate based coordination polymers: theoretical prediction via DFT study. <i>Dalton Transactions</i> , 2021, 50, 270-278.	3.3	8
66	A first exploration of isostructurality in transition metal nitroprussides: X-ray analysis, magnetic properties and DFT calculations. <i>CrystEngComm</i> , 2021, 23, 1158-1171.	2.6	3
67	Ligand structure-driven self-assembly of Zn(NCS) ₂ with a carbohydrazone ligand: A possible intermediate towards a [2D \cdots 2] metallic grid. <i>Journal of Molecular Structure</i> , 2021, 1225, 129269.	3.6	4
68	A supramolecular 3D structure constructed from a new metal chelate self-assembled from Sn(NCS) ₂ and phenyl(pyridin-2-yl)methylenepicolinohydrazide. <i>Journal of Molecular Structure</i> , 2021, 1224, 129188.	3.6	8
69	Energetically significant cooperative π -stacked ternary assemblies in Ni(II) phenanthroline compounds involving discrete water clusters: Anticancer activities and theoretical studies. <i>Journal of Molecular Structure</i> , 2021, 1229, 129486.	3.6	17
70	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. <i>Inorganica Chimica Acta</i> , 2021, 516, 120082.	2.4	16
71	A tetrameric udd type water cluster encapsulated in a dinuclear vanadium(V) Schiff base complex and its role in the formation of supramolecular assemblies: A joint experimental and theoretical study. <i>Inorganica Chimica Acta</i> , 2021, 515, 120057.	2.4	13
72	Existence of stronger $C\cdots N$ (chelate ring) interaction compared to $C\cdots N$ (arene) interactions in the supramolecular assembly of dinuclear iron(III) Schiff base complexes: A theoretical insight. <i>Inorganica Chimica Acta</i> , 2021, 516, 120081.	2.4	9

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73	Unprecedented [d9]Cu ⁺ [d10]Au coinage bonding interactions in {Cu(NH ₃) ₄ [Au(CN) ₂]} ⁺ [Au(CN) ₂] ⁻ salt. <i>Chemical Communications</i> , 2021, 57, 7268-7271.	4.1	8
74	Anion-dependent structural variations and charge transport property analysis of 4-(3-pyridyl)-4,2,6-terpyridinium salts. <i>CrystEngComm</i> , 2021, 23, 3569-3581.	2.6	5
75	Insight into non-covalent interactions in two triamine-based mononuclear iron(III) Schiff base complexes with special emphasis on the formation of Br ⁻ halogen bonding. <i>CrystEngComm</i> , 2021, 23, 1578-1587.	2.6	8
76	Ultrashort H ⁺ ⋯H ⁺ intermolecular distance in a supramolecular system in the solid state. <i>Chemical Communications</i> , 2021, 57, 7112-7115.	4.1	4
77	Supramolecular assemblies involving biologically relevant antiparallel π -stacking and unconventional solvent driven structural topology in maleato and fumarato bridged Zn(II) coordination polymers: antiproliferative evaluation and theoretical studies. <i>New Journal of Chemistry</i> , 2021, 45, 13040-13055.	2.8	9
78	Dual role of silver in a fluorogenic Ni-squaraine probe based on Ag(I) interactions. <i>Dalton Transactions</i> , 2021, 50, 9367-9371.	3.3	2
79	An experimental and theoretical exploration of supramolecular interactions and photoresponse properties of two Ni(II) complexes. <i>New Journal of Chemistry</i> , 2021, 45, 12108-12119.	2.8	8
80	Synthesis and characterization of a mononuclear zinc(II) Schiff base complex: on the importance of C ⁺ ⋯H ⁻ interactions. <i>RSC Advances</i> , 2021, 11, 30148-30155.	3.6	13
81	Theoretical study of spodium bonding in the active site of three Zn-proteins and several model systems. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16888-16896.	2.8	12
82	H-Bonds, π -Stacking and (Water)O-H/ π Interactions in (μ -4-EDTA)Bis(Imidazole) Dicopper(II) Dihydrate. <i>Crystals</i> , 2021, 11, 48.	2.2	4
83	Crystal engineering with pyrazolyl-thiazole derivatives: structure-directing role of π -stacking and π -hole interactions. <i>CrystEngComm</i> , 2021, 23, 3276-3287.	2.6	21
84	A theoretical insight on the anion-anion interactions observed in the solid state structure of a hetero-trinuclear complex. <i>CrystEngComm</i> , 2021, 23, 1429-1438.	2.6	11
85	On the importance of R ₃ C ⁺ N tetrel bonding interactions in the solid state of a dinuclear zinc complex with a tetradentate Schiff base ligand. <i>CrystEngComm</i> , 2021, 23, 3391-3397.	2.6	8
86	Differentiating intramolecular spodium bonds from coordination bonds in two polynuclear zinc(II) Schiff base complexes. <i>CrystEngComm</i> , 2021, 23, 2703-2710.	2.6	39
87	A convenient access to fluorophosphonium triflate salts by electrophilic fluorination and anion exchange. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 2854-2864.	6.0	7
88	Biological halogen bonds in protein-ligand complexes: a combined QTAIM and NCIPlot study in four representative cases. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 6858-6864.	2.8	10
89	Glutamate carboxypeptidase II as a model system for designing host-guest units: a theoretical approach. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 7816-7821.	2.8	1
90	Spodium bonding in five coordinated Zn(II): a new player in crystal engineering?. <i>CrystEngComm</i> , 2021, 23, 3084-3093.	2.6	33

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91	Biologically relevant and energetically significant cooperative ternary $(\text{H}_2\text{O})_{21}$ clusters in isostructural 2,5-pyridine dicarboxylato Co(II) and Zn(II) phenanthroline compounds: antiproliferative evaluation and theoretical studies. <i>New Journal of Chemistry</i> , 2021, 45, 3699-3715.	2.8	13
92	Synthesis of Ni(II)-Mn(II) complexes using a new mononuclear Ni(II) complex of an unsymmetrical N_2O_3 donor ligand: structures, magnetic properties and catalytic oxidase activity. <i>Dalton Transactions</i> , 2021, 50, 4686-4699.	3.3	25
93	Iodonium complexes of the tertiary amines quinuclidine and 1-ethylpiperidine. <i>Dalton Transactions</i> , 2021, 50, 8297-8301.	3.3	16
94	Nickel(II) complexes based on dithiolate-polyamine binary ligand systems: crystal structures, Hirshfeld surface analysis, theoretical study, and catalytic activity study on photocatalytic hydrogen generation. <i>Dalton Transactions</i> , 2021, 50, 5632-5643.	3.3	13
95	π -Hole spodium bonding in tri-coordinated Hg(II) complexes. <i>Dalton Transactions</i> , 2021, 50, 7545-7553.	3.3	14
96	A theoretical insight into the formation of chalcogen bonding (ChB) interactions involving coordinated DMSO molecules as π -hole donors and benzoate groups as π -hole acceptors in a dinuclear copper(II) complex. <i>CrystEngComm</i> , 2021, 23, 5087-5096.	2.6	12
97	Nucleophilic Iodonium Interactions (NIIs) in 2-coordinate iodine(I) and silver(I) complexes. <i>Chemical Communications</i> , 2021, 57, 5094-5097.	4.1	13
98	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. <i>New Journal of Chemistry</i> , 2021, 45, 19928-19940.	2.8	22
99	Insight into the formation of H-bonds propagating the monomeric zinc complexes of a tridentate reduced Schiff base to form an infinite chain. <i>CrystEngComm</i> , 2021, 23, 1918-1928.	2.6	6
100	Bifurcated Halogen Bonding Involving Two Rhodium(I) Centers as an Integrated π -Hole Acceptor. <i>Jacs Au</i> , 2021, 1, 354-361.	7.9	39
101	Weak Interactions in Cocrystals of Isoniazid with Glycolic and Mandelic Acids. <i>Crystals</i> , 2021, 11, 328.	2.2	8
102	Catecholase-Like Activity and Theoretical Study in Solid State of a New Ru(III)-Schiff Base Complex. <i>Acta Chimica Slovenica</i> , 2021, 68, 212-221.	0.6	2
103	Utility of Three-Coordinate Silver Complexes Toward the Formation of Iodonium Ions. <i>Inorganic Chemistry</i> , 2021, 60, 5383-5390.	4.0	24
104	Synthesis, characterization, DNA binding ability, <i>in vitro</i> cytotoxicity, electrochemical properties and theoretical studies of copper(II) carboxylate complexes. <i>Inorganica Chimica Acta</i> , 2021, 518, 120235.	2.4	13
105	A nucleophilic iodine in a halogen-bonded Iodonium complex manifests an unprecedented $\text{I}^+\cdots\text{Ag}^+$ interaction. <i>CheM</i> , 2021, 7, 948-958.	11.7	32
106	Cd(II) coordination polymer of fumaric acid and pyridyl-hydrazide Schiff base: Structure, photoconductivity and theoretical interpretation. <i>Inorganica Chimica Acta</i> , 2021, 518, 120253.	2.4	17
107	Azine Steric Hindrances Switch Halogen Bonding to $\text{N}^{\delta-}\cdots\text{N}^{\delta+}$ Arylation upon Interplay with π -Hole Donating Haloarene nitriles. <i>Chemistry - an Asian Journal</i> , 2021, 16, 1445-1455.	3.3	9
108	Short $\text{X}\cdots\text{N}$ Halogen Bonds With Hexamethylenetetraamine as the Acceptor. <i>Frontiers in Chemistry</i> , 2021, 9, 623595.	3.6	7

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109	Using Room Temperature Phosphorescence of Gold(I) Complexes for PAHs Sensing. <i>Molecules</i> , 2021, 26, 2444.	3.8	7
110	Dicopper(II)-EDTA Chelate as a Bicephalic Receptor Model for a Synthetic Adenine Nucleoside. <i>Pharmaceuticals</i> , 2021, 14, 426.	3.8	3
111	Anionâ€¦â€¦Anion Coinage Bonds: The Case of Tetrachloridoaurate. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 14385-14389.	13.8	46
112	Spodium bonding and other non-covalent interactions assisted supramolecular aggregation in a new mercury(II) complex of a nicotinohydrazide derivative. <i>Inorganica Chimica Acta</i> , 2021, 519, 120279.	2.4	25
113	Anionâ€¦â€¦Anion Coinage Bonds: The Case of Tetrachloridoaurate. <i>Angewandte Chemie</i> , 2021, 133, 14506-14510.	2.0	4
114	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. <i>Inorganica Chimica Acta</i> , 2021, 521, 120298.	2.4	8
115	Tri- and pentanuclear CuIIâ€¦CdII complexes of N2O2 donor ligands with the variation of carboxylate coligands: Structural elucidation and theoretical study. <i>Inorganica Chimica Acta</i> , 2021, 521, 120351.	2.4	1
116	Ligand Steric Hindrances Switch Bridging ($\frac{1}{4}$ -Iâ€¦O,O to Two-Center Iâ€¦O Halogen-Bonding Mode in the Assembly of Diketonate Copper(II) Species. <i>Crystal Growth and Design</i> , 2021, 21, 4073-4082.	3.0	5
117	A new coordination polymer constructed from Pb(NO3)2 and a benzylideneisonicotinohydrazide derivative: Coordination-induced generation of a π -hole towards a tetrel-bonding stabilized structure. <i>Journal of Molecular Structure</i> , 2021, 1234, 130139.	3.6	11
118	Diastereoselective Amplification of a Mechanically Chiral [2]Catenane. <i>Journal of the American Chemical Society</i> , 2021, 143, 11957-11962.	13.7	29
119	Charge Assisted S/Se Chalcogen Bonds in SAM Riboswitches: A Combined PDB and ab Initio Study. <i>ACS Chemical Biology</i> , 2021, 16, 1701-1708.	3.4	13
120	Diaryliodonium Tetrachloroplatinates(II): Recognition of a Trifurcated Metal-Involving $\frac{1}{4}$ -Iâ€¦(Cl,Cl,Pt) Halogen Bond. <i>Crystal Growth and Design</i> , 2021, 21, 5360-5372.	3.0	23
121	Spodium Bonds in Biological Systems: Expanding the Role of Zn in Protein Structure and Function. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3945-3954.	5.4	21
122	Molecular Electrostatic Potential and Noncovalent Interactions in Derivatives of Group 8 Elements. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20723-20727.	13.8	58
123	1-Ethyluracil, a New Scaffold for Preparing Multicomponent Forms: Synthesis, Characterization, and Computational Studies. <i>Crystal Growth and Design</i> , 2021, 21, 4857-4870.	3.0	2
124	Molecular Electrostatic Potential and Noncovalent Interactions in Derivatives of Group 8 Elements. <i>Angewandte Chemie</i> , 2021, 133, 20891-20895.	2.0	9
125	Noble metals in polyoxometalates. <i>Inorganica Chimica Acta</i> , 2021, 523, 120410.	2.4	10
126	Bifunctional Fluorophosphonium Triflates as Intramolecular Frustrated Lewis Pairs: Reversible CO ₂ Sequestration and Binding of Carbonyls, Nitriles and Acetylenes. <i>Chemistry - A European Journal</i> , 2021, 27, 13709-13714.	3.3	9

#	ARTICLE	IF	CITATIONS
127	Importance of Anion- π Interactions in RNA GAAA and GGAG Tetraloops: A Combined MD and QM Study. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6624-6633.	5.3	5
128	Solvent driven structural topologies involving unconventional O H(methanol)- π contact and anti-cooperative HB π -anion- π HB assemblies with unusual enclathration of dual guest (H ₂ O) ₄ cores in Mn(II) and Ni(II) coordination compounds: Antiproliferative evaluation and theoretical studies. <i>Polyhedron</i> , 2021, 210, 115503.	2.2	2
129	Unconventional π -hole and Semi-coordination regium bonding interactions directed supramolecular assemblies in pyridinedicarboxylato bridged polymeric Cu(II) Compounds: Antiproliferative evaluation and theoretical studies. <i>Inorganica Chimica Acta</i> , 2021, 525, 120461.	2.4	10
130	Anion- π ... π -Anion Interactions Involving π -Holes of Perrhenate, Pertechnetate and Permanganate Anions. <i>ChemPhysChem</i> , 2021, 22, 2281-2285.	2.1	60
131	Frustrated Lewis Pairs based on Carbon- π -Carbon+ tetrel bonds: A DFT study. Mar \tilde{A} a de las Nieves Pi \tilde{A} a[a], Antonio Frontera[a], Tidde. J. Mooibroek[b],* and Antonio Bauz \tilde{A} i*[a]. <i>ChemPhysChem</i> , 2021, 22, 2478-2483.	2.1	3
132	An insight into the supramolecular interactions in two linear polyvanadates. <i>Journal of Molecular Structure</i> , 2021, 1242, 130681.	3.6	2
133	Uracil Derivatives for Halogen-Bonded Cocrystals. <i>International Journal of Molecular Sciences</i> , 2021, 22, 10663.	4.1	7
134	Benzoato bridged dinuclear Mn(II) and Cu(II) compounds involving guest chlorobenzoates and dimeric paddle wheel supramolecular assemblies: Antiproliferative evaluation and theoretical studies. <i>Polyhedron</i> , 2021, 208, 115409.	2.2	9
135	Solvothermal self assembly of three lanthanide(III)-succinates: Crystal structure, topological analysis and DFT calculations on water channel. <i>Journal of Molecular Structure</i> , 2021, 1245, 131094.	3.6	12
136	Supramolecular, spectroscopic and computational analysis of weak interactions in some thiosemicarbazones derived from 5-acetylbarbituric acid. <i>Journal of Molecular Structure</i> , 2021, 1245, 131031.	3.6	1
137	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. <i>Journal of Molecular Structure</i> , 2021, 1245, 131038.	3.6	8
138	Metalloid Chalcogen- π -pnictogen π -hole bonding competition in stibanyl telluranes. <i>Journal of Organometallic Chemistry</i> , 2021, 954-955, 122092.	1.8	5
139	Selenium chalcogen bonds are involved in protein- π carbohydrate recognition: a combined PDB and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17656-17662.	2.8	14
140	Molecular 1,1- π -bifunctional mixed-valence P π -P compounds, enabled through metal complexation. <i>Dalton Transactions</i> , 2021, 50, 2131-2137.	3.3	4
141	Biologically relevant unusual cooperative assemblies and fascinating infinite crown-like supramolecular nitrate-water hosts involving guest complex cations in bipyridine and phenanthroline-based Cu(II) coordination compounds: antiproliferative evaluation and theoretical studies. <i>New Journal of Chemistry</i> , 2021, 45, 8269-8282.	2.8	14
142	Electron belt-to- π -hole switch of noncovalently bound iodine atoms in dithiocarbamate metal complexes. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 2505-2517.	6.0	25
143	Phenoxido mediated antiferromagnetic and azide mediated ferromagnetic coupling in two dinuclear ferromagnetic nickel complexes with isomeric Schiff bases: a theoretical insight on the pathway of magnetic interaction. <i>CrystEngComm</i> , 2021, 23, 1942-1952.	2.6	8
144	Supramolecular network of a framework material supported by the anion- π linkage of Keggin-type heteropolyoxotungstates: experimental and theoretical insights. <i>Dalton Transactions</i> , 2021, 50, 1895-1900.	3.3	31

#	ARTICLE	IF	CITATIONS
145	A combined theoretical and CSD perspective on σ -hole interactions with tetrels, pnictogens, chalcogens, halogens, and noble gases. , 2021, , 119-155.		4
146	Change in molecular shapes of the trinuclear CuI ₂ ZnII complexes on Schiff base reduction: structural and theoretical investigations. CrystEngComm, 2021, 23, 4848-4856.	2.6	3
147	Synthesis and crystal structure of the simultaneous binding of Ni(II) cation and chloride by the protonated 2,4,6 tris-(2-pyridyl)-1,3,5 triazine ligand: theoretical investigations of anion- σ -hole and hydrogen bonding interactions. New Journal of Chemistry, 2021, 45, 11689-11696.	2.8	13
148	On the nature of recurrent Au σ -hole motifs in tris(2,2'-bipyridine)M(II) (M = Fe, Co and Ni) dicyanoaurate salts: X-ray analysis and theoretical rationalization. Dalton Transactions, 2021, 50, 16954-16960.	3.3	4
149	Hydrogen bond mediated intermolecular magnetic coupling in mononuclear high spin iron(III) Schiff base complexes: synthesis, structure and magnetic study with theoretical insight. RSC Advances, 2021, 11, 3315-3323.	3.6	11
150	Understanding the planar conformations in diarylsubstituted heteroarenes: structural and theoretical insights. CrystEngComm, 2021, 23, 3144-3151.	2.6	7
151	Highly polar stacking interactions wrap inorganics in organics: lone-pair σ -hole interactions between the PdO ₄ core and electron-deficient arenes. Inorganic Chemistry Frontiers, 2021, 8, 4965-4975.	6.0	15
152	Coordination versus σ -bonding in dinuclear Zn(II) and Cd(II) complexes with a dithiophosphate ligand. New Journal of Chemistry, 2021, 45, 19402-19415.	2.8	17
153	Macrocyclic complexes based on [N σ -N] σ -halogen bonds. Chemical Communications, 2021, 57, 12464-12467.	4.1	12
154	On the Importance of σ -Hole Interactions in Crystal Structures. Crystals, 2021, 11, 1205.	2.2	48
155	Novel σ -isostructuralism in metal complexes with 1-methylimidazole: crystal structures, energy calculations and magnetic properties. Dalton Transactions, 2021, 50, 17029-17040.	3.3	1
156	A homonuclear σ -system with a singlet carbene-type σ and a nucleophilic σ^2 phosphorus σ the first use in P-heterocyclic synthesis. Dalton Transactions, 2021, 50, 17892-17896.	3.3	2
157	Charge Assisted Hydrogen Bonded Assemblies and Unconventional O σ -O σ 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.	3.6	6
158	On the Importance of Pnictogen and Chalcogen Bonding Interactions in Supramolecular Catalysis. International Journal of Molecular Sciences, 2021, 22, 12550.	4.1	40
159	On the Importance of Halogen Bonding Interactions in Two X-ray Structures Containing All Four (F, Cl, Br, I) Halogens. Crystals, 2021, 11, 1205.	2.2	29
160	Coordination complexes of zinc and manganese based on pyridine-2,5-dicarboxylic acid N-oxide: DFT studies and antiproliferative activities consideration. RSC Advances, 2021, 11, 37403-37412.	3.6	7
161	Osme bond: anisotropic distribution of electron density in action. Acta Crystallographica Section A: Foundations and Advances, 2021, 77, C800-C800.	0.1	2
162	Gold(III) as an effective electrophilic site, namely coinage bond donor: assembly of AuCl ₄ units into supramolecular anionic polymers. Acta Crystallographica Section A: Foundations and Advances, 2021, 77, C214-C214.	0.1	1

#	ARTICLE	IF	CITATIONS
163	Novel Polymorphic Cocrystals of the Non-Steroidal Anti-Inflammatory Drug Niflumic Acid: Expanding the Pharmaceutical Landscape. <i>Pharmaceutics</i> , 2021, 13, 2140.	4.5	9
164	Synthesis, structural and DFT interpretation of a Schiff base assisted Mn(III) derivative. <i>Journal of Molecular Structure</i> , 2020, 1199, 126985.	3.6	3
165	Synthesis, reactivity, X-ray characterization and docking studies of N7/N9-(2-pyrimidyl)-adenine derivatives. <i>Journal of Inorganic Biochemistry</i> , 2020, 203, 110879.	3.5	6
166	Halogen interactions in dinuclear copper(II) 2,4-dibromophenoxyacetate " crystal structure and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2020, 1202, 127227.	3.6	5
167	Ionpair- π interactions favor cell penetration of arginine/tryptophan-rich cell-penetrating peptides. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020, 1862, 183098.	2.6	51
168	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. <i>Inorganica Chimica Acta</i> , 2020, 501, 119233.	2.4	26
169	Through-space π - π Effect between the Bridging Oxygen Atoms in Diepoxybenzo[de]isothiochromene Derivatives. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 156-161.	2.4	7
170	Zn(II) and Co(II) derivatives anchored with scorpionate precursor: Antiproliferative evaluation in human cancer cell lines. <i>Journal of Inorganic Biochemistry</i> , 2020, 202, 110881.	3.5	4
171	A combined experimental and computational study of a supramolecular assembly based on cationic zinc(II)-ethanesulfonate. <i>Journal of Molecular Structure</i> , 2020, 1202, 127206.	3.6	1
172	Supramolecular assembly of a 2D coordination polymer bearing pyridine-N-oxide-2,5-dicarboxylic acid and copper ion: X-ray crystallography and DFT calculations. <i>Journal of Molecular Structure</i> , 2020, 1202, 127243.	3.6	22
173	On the Role of Water as a Catalyst in Prebiotic Chemistry. <i>ChemPhysChem</i> , 2020, 21, 313-320.	2.1	8
174	Combined experimental and computational studies on preferential CO ₂ adsorption over a zinc-based porous framework solid. <i>New Journal of Chemistry</i> , 2020, 44, 1806-1816.	2.8	4
175	Molecular and supramolecular recognition patterns in ternary copper(II) or zinc(II) complexes with selected rigid-planar chelators and a synthetic adenine-nucleoside. <i>Journal of Inorganic Biochemistry</i> , 2020, 203, 110920.	3.5	5
176	Influence of 2-Amino-4-methylpyridine and 2-Aminopyrimidine Ligands on the Malonic Acid-Cu(II) System: Insights through Supramolecular Interactions and Photoresponse Properties. <i>ACS Omega</i> , 2020, 5, 460-470.	3.5	7
177	Self-assembly of amphiphilic aryl-squaramides in water driven by dipolar π - π interactions. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 888-894.	2.8	16
178	Metal-organic architectures driven by a multifunctional 6-aminouracil spacer: structures, noncovalent interactions, and conductivity. <i>CrystEngComm</i> , 2020, 22, 829-840.	2.6	7
179	The Effect of Guest Metal Ions on the Reduction Potentials of Uranium(VI) Complexes: Experimental and Theoretical Investigations. <i>Chemistry - A European Journal</i> , 2020, 26, 1612-1623.	3.3	19
180	Supramolecular architecture constructed from the hemidirected lead(II) complex with N'-(4-hydroxybenzylidene)isonicotinohydrazide. <i>Inorganica Chimica Acta</i> , 2020, 502, 119350.	2.4	25

#	ARTICLE	IF	CITATIONS
181	Energetically significant unconventional O-H... π contacts involving discrete guest (H ₂ O) ₈ clusters in a fumarate bridged polymeric supramolecular host of Ni(II) phenanthroline: Antiproliferative evaluation and theoretical studies. <i>Polyhedron</i> , 2020, 176, 114266.	2.2	23
182	Halogen and Chalcogen Bond Energies Evaluated Using Electron Density Properties. <i>ChemPhysChem</i> , 2020, 21, 26-31.	2.1	61
183	π -Hole noble gas bonding interactions: Insights from theory and experiment. <i>Coordination Chemistry Reviews</i> , 2020, 404, 213112.	18.8	83
184	Tetrel Bonding Interactions Involving Carbon at Work: Recent Advances in Crystal Engineering and Catalysis. <i>Journal of Carbon Research</i> , 2020, 6, 60.	2.7	12
185	Intramolecular Spodium Bonds in Zn(II) Complexes: Insights from Theory and Experiment. <i>International Journal of Molecular Sciences</i> , 2020, 21, 7091.	4.1	41
186	Reaction of Cu(II) Chelates with Uranyl Nitrate to Form a Coordination Complex or H-Bonded Adduct: Experimental Observations and Rationalization by Theoretical Calculations. <i>Inorganic Chemistry</i> , 2020, 59, 15848-15861.	4.0	23
187	Intermolecular interactions in antipyrine-like derivatives 2-halo-N-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)benzamides: X-ray structure, Hirshfeld surface analysis and DFT calculations. <i>New Journal of Chemistry</i> , 2020, 44, 19541-19554.	2.8	23
188	Supramolecular assemblies involving salt bridges: DFT and X-ray evidence of bipolarity. <i>CrystEngComm</i> , 2020, 22, 8171-8181.	2.6	21
189	Recurrent π (arene)- π (chelate ring) motifs in four trinuclear CuII ₂ MII (M = Cd/Zn) complexes derived from an unsymmetrical N ₂ O ₂ donor ligand: structural and theoretical investigations. <i>CrystEngComm</i> , 2020, 22, 7673-7683.	2.6	7
190	Unravelling the electronic nature of C \cdots F \cdots O \cdots C non-covalent interaction in proteins and small molecules in the solid state. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25704-25711.	2.8	9
191	Naphthalenediimides with Cyclic Oligochalcogenides in Their Core. <i>Chemistry - A European Journal</i> , 2020, 26, 14059-14063.	3.3	5
192	Supramolecular architectures of Mn(NCS) ₂ complexes with N'-(1-(pyridin-4-yl)ethylidene)picolinohydrazide and N'-(phenyl(pyridin-4-yl)methylene)isonicotinohydrazide. <i>Polyhedron</i> , 2020, 190, 114776.	2.2	9
193	Novel Pb(II) Complexes: X-Ray Structures, Hirshfeld Surface Analysis and DFT Calculations. <i>Crystals</i> , 2020, 10, 568.	2.2	9
194	A new spodium bond driven coordination polymer constructed from mercury(μ) ₂ azide and 1,2-bis(pyridin-2-ylmethylene)hydrazine. <i>New Journal of Chemistry</i> , 2020, 44, 21100-21107.	2.8	21
195	Interconvertible Hydrochlorothiazide-Caffeine Multicomponent Pharmaceutical Materials: A Solvent Issue. <i>Crystals</i> , 2020, 10, 1088.	2.2	13
196	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. <i>Polyhedron</i> , 2020, 191, 114809.	2.2	20
197	Raise the anchor! Synthesis, X-ray and NMR characterization of 1,3,5-triazinanes with an axial <i>tert</i> -butyl group. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 8386-8394.	2.8	5
198	In-vitro prediction of the membranotropic action of emerging organic contaminants using a liposome-based multidisciplinary approach. <i>Science of the Total Environment</i> , 2020, 738, 140096.	8.0	7

#	ARTICLE	IF	CITATIONS
199	Recurrent π - π stacking motifs in three new 4,5-dihydropyrazolyl-thiazole-coumarin hybrids: X-ray characterization, Hirshfeld surface analysis and DFT calculations. <i>New Journal of Chemistry</i> , 2020, 44, 14592-14603.	2.8	54
200	Noble Gas Bonding Interactions Involving Xenon Oxides and Fluorides. <i>Molecules</i> , 2020, 25, 3419.	3.8	21
201	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. <i>Polyhedron</i> , 2020, 189, 114711.	2.2	0
202	A theoretical insight into non-covalent supramolecular interactions in the solid state structures of two octahedral iron(III) complexes. <i>CrystEngComm</i> , 2020, 22, 5731-5742.	2.6	14
203	Synthesis, X-ray characterization and theoretical study of 3a,6:7,9a-diepoxybenzo[de]isoquinoline derivatives: on the importance of F \cdots O interactions. <i>New Journal of Chemistry</i> , 2020, 44, 20167-20180.	2.8	7
204	On the supramolecular properties of neutral, anionic and cationic cadmium complexes harvested from dithiolate-polyamine binary ligand systems. <i>CrystEngComm</i> , 2020, 22, 8023-8035.	2.6	10
205	Oxalato bridged coordination polymer of manganese(III) involving unconventional O \cdots H-hole(nitrile) and antiparallel nitrile \cdots nitrile contacts: antiproliferative evaluation and theoretical studies. <i>New Journal of Chemistry</i> , 2020, 44, 20021-20038.	2.8	22
206	Methylene spacer regulated variation in supramolecular assembly of zinc(II) dicyanamide complexes with reduced Schiff base ligands: synthesis, structure and DFT study. <i>CrystEngComm</i> , 2020, 22, 6876-6885.	2.6	15
207	Semicoordination Bond Breaking and Halogen Bond Making Change the Supramolecular Architecture of Metal-Containing Aggregates. <i>Crystal Growth and Design</i> , 2020, 20, 6956-6965.	3.0	38
208	π - and π -Hole Interactions. <i>Crystals</i> , 2020, 10, 721.	2.2	9
209	Regioselective Bonds Are Involved in Protein-Gold Binding. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8259-8263.	4.6	25
210	A facile biomimetic catalytic activity through hydrogen atom abstraction by the secondary coordination sphere in manganese(III) complexes. <i>Dalton Transactions</i> , 2020, 49, 14216-14230.	3.3	12
211	Tetrel Bonding and Other Non-Covalent Interactions Assisted Supramolecular Aggregation in a New Pb(II) Complex of an Isonicotinohydrazide. <i>Molecules</i> , 2020, 25, 4056.	3.8	25
212	DFT Analysis of Uncommon π - π -H-Bond Array Interaction in a New Pterostilbene/Theophylline Cocrystal. <i>Crystal Growth and Design</i> , 2020, 20, 6691-6698.	3.0	19
213	Recurrent motifs in pharmaceutical cocrystals involving glycolic acid: X-ray characterization, Hirshfeld surface analysis and DFT calculations. <i>CrystEngComm</i> , 2020, 22, 6674-6689.	2.6	19
214	Crystal structures of <i>N</i> - ⁶ -modified-amino acid nucleobase analogs(III): adenine-valeric acid, adenine-hexanoic acid and adenine-gabapentine. <i>New Journal of Chemistry</i> , 2020, 44, 12236-12246.	2.8	5
215	Sildenafil-Resorcinol Cocrystal: XRPD Structure and DFT Calculations. <i>Crystals</i> , 2020, 10, 1126.	2.2	15
216	Radical-radical chalcogen bonds: CSD analysis and DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12757-12765.	2.8	10

#	ARTICLE	IF	CITATIONS
217	Covalent and Non-covalent Noble Gas Bonding Interactions in XeFn Derivatives (n = 2-6): A Combined Theoretical and ICSD Analysis. <i>Frontiers in Chemistry</i> , 2020, 8, 395.	3.6	22
218	Complexes of BiCl ₃ with hydrazone derived ligands: a Möbius-like discrete metal chelate versus a salt-like porous polymeric structure. <i>New Journal of Chemistry</i> , 2020, 44, 9429-9437.	2.8	5
219	Coordination polymers of manganese(II), cobalt(II), nickel(II) and cadmium(II) decorated with rigid pyrazine-2,3-dicarboxylic acid linker: Synthesis, structural diversity, DFT study and magneto-luminescence properties. <i>Polyhedron</i> , 2020, 187, 114629.	2.2	13
220	Quantifying Intramolecular Halogen Bonds in Nucleic Acids: A Combined Protein Data Bank and Theoretical Study. <i>ACS Chemical Biology</i> , 2020, 15, 1942-1948.	3.4	18
221	Selective functionalisation of aromatic alcohols with supramolecularly regulated gold(scp) catalysts. <i>Organic Chemistry Frontiers</i> , 2020, 7, 1626-1634.	4.5	9
222	Metal removal from the secondary building unit of bio-MOF-1 by adenine N6-alkylation while retaining the overall 3D porous topology. <i>CrystEngComm</i> , 2020, 22, 4201-4205.	2.6	2
223	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. <i>Journal of Molecular Structure</i> , 2020, 1217, 128398.	3.6	7
224	Selective Metal-Ligand Bond-Breaking Driven by Weak Intermolecular Interactions: From Metamagnetic Mn(III)-Monomer to Hexacyanoferrate(II)-Bridged Metamagnetic Mn ₂ Fe Trimer. <i>Inorganic Chemistry</i> , 2020, 59, 8487-8497.	4.0	5
225	Spodium Bonds: Noncovalent Interactions Involving Group 12 Elements. <i>Angewandte Chemie</i> , 2020, 132, 17635-17640.	2.0	21
226	Spodium Bonds: Noncovalent Interactions Involving Group 12 Elements. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 17482-17487.	13.8	136
227	Halogen Bonds in Protein Nucleic Acid Recognition. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4744-4752.	5.3	25
228	Role of Imidazole Co-Ligand in the Supramolecular Network of a Co(II) Complex with Sulfadiazine: Crystal Structure, Hirshfeld Surface Analysis and Energetic Calculations. <i>ChemistrySelect</i> , 2020, 5, 6331-6338.	1.5	9
229	Engineering Crystals Using sp ³ Centred Tetrel Bonding Interactions. <i>Chemistry - A European Journal</i> , 2020, 26, 10126-10132.	3.3	28
230	Exploration of Br [⋯] O halogen bonding interactions in dinuclear vanadium(V) complexes with Schiff base ligands. <i>Polyhedron</i> , 2020, 187, 114676.	2.2	18
231	One-Pot Route to X-perfluoroarenes (X = Br, I) Based on Fe ^{III} -Assisted C-F Functionalization and Utilization of These Arenes as Building Blocks for Crystal Engineering Involving Halogen Bonding. <i>Crystal Growth and Design</i> , 2020, 20, 5908-5921.	3.0	30
232	π-Hole-π-π-π _z [Pt ^{II}] Interactions with Electron-Deficient Arenes Enhance the Phosphorescence of Pt ^{II} -Based Luminophores. <i>Inorganic Chemistry</i> , 2020, 59, 9308-9314.	4.0	39
233	Intramolecular sp ² -sp ³ Disequalization of Chemically Identical Sulfonamide Nitrogen Atoms: Single Crystal X-Ray Diffraction Characterization, Hirshfeld Surface Analysis and DFT Calculations of N-Substituted Hexahydro-1,3,5-Triazines. <i>Crystals</i> , 2020, 10, 369.	2.2	4
234	Novel Cd (II) Coordination Polymers Afforded with EDTA or Trans-1,2-Cdta Chelators and Imidazole, Adenine, or 9-(2-Hydroxyethyl) Adenine Coligands. <i>Crystals</i> , 2020, 10, 391.	2.2	2

#	ARTICLE	IF	CITATIONS
235	Asymmetric [Nâ€“â€“N] ⁺ halonium complexes. <i>Chemical Communications</i> , 2020, 56, 8428-8431.	4.1	41
236	Synthesis, X-ray characterization and regium bonding interactions of a trichlorido(1-hexylcytosine)gold(III) complex. <i>Chemical Communications</i> , 2020, 56, 3524-3527.	4.1	28
237	Not Only Hydrogen Bonds: Other Noncovalent Interactions. <i>Crystals</i> , 2020, 10, 180.	2.2	289
238	Supramolecular and theoretical perspectives of 2,2':6''-2''-terpyridine based Ni(II) and Cu(II) complexes: on the importance of Câ€“Hâ€“Cl and Iâ€“I interactions. <i>New Journal of Chemistry</i> , 2020, 44, 7310-7318.	2.8	22
239	Supramolecular Assembly of Metal Complexes by (Aryl)â€“â€“d[Pt(II)] Halogen Bonds. <i>Chemistry - A European Journal</i> , 2020, 26, 7692-7701.	3.3	54
240	Binuclear and tetranuclear Zn(II) complexes with thiosemicarbazones: synthesis, X-ray crystal structures, ATP-sensing, DNA-binding, phosphatase activity and theoretical calculations. <i>RSC Advances</i> , 2020, 10, 12735-12746.	3.6	9
241	Charge assisted halogen and pnictogen bonds: insights from the Cambridge Structural Database and DFT calculations. <i>CrystEngComm</i> , 2020, 22, 7162-7169.	2.6	21
242	Charge-assisted hydrogen bond and nitrileâ€“nitrile interaction directed supramolecular associations in Cu(II) and Mn(II) coordination complexes: anticancer, hematotoxicity and theoretical studies. <i>New Journal of Chemistry</i> , 2020, 44, 5473-5488.	2.8	34
243	A late appearing polymorph of nutraceutical pterostilbene. <i>CrystEngComm</i> , 2020, 22, 4680-4684.	2.6	10
244	Adipato bridged novel hexanuclear Cu(II) and polymeric Co(II) coordination compounds involving cooperative supramolecular assemblies and encapsulated guest water clusters in a square grid host: antiproliferative evaluation and theoretical studies. <i>Dalton Transactions</i> , 2020, 49, 9863-9881.	3.3	27
245	Pnictogen-bonding catalysis: brevetoxin-type polyether cyclizations. <i>Chemical Science</i> , 2020, 11, 7086-7091.	7.4	62
246	Diminishing accessibility of electrophilic nickel(II) centres due to incorporation of a methylene spacer in the pendant side arm of a series of heterotrinnuclear nickel(II)/sodium complexes: a DFT study using a homodesmotic equation. <i>CrystEngComm</i> , 2020, 22, 2970-2977.	2.6	10
247	Unconventional DNA-relevant Iâ€“stacked hydrogen bonded arrays involving supramolecular guest benzoate dimers and cooperative anionâ€“anion contacts in coordination compounds of Co(II) and Zn(II) phenanthroline: experimental and theoretical studies. <i>New Journal of Chemistry</i> , 2020, 44, 4504-4518.	2.8	24
248	Halogenâ€“halogen interactions in decahalo-closo-carboranes: CSD analysis and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 6122-6130.	2.8	12
249	A combined experimental and theoretical study on an ionic cobalt(III/II) complex with a Schiff base ligand. <i>Polyhedron</i> , 2020, 182, 114432.	2.2	5
250	Synthesis, X-ray Characterization and Density Functional Theory (DFT) Studies of Two Polymorphs of the Î±,Î±,Î±,Î± Isomer of Tetra-p-Iodophenyl Tetramethyl Calix[4]pyrrole: On the Importance of Halogen Bonds. <i>Molecules</i> , 2020, 25, 285.	3.8	3
251	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. <i>Polyhedron</i> , 2020, 179, 114374.	2.2	13
252	DFT analysis of supra-molecular assemblies of substituted 4H-pyran derivatives. <i>Journal of Molecular Structure</i> , 2020, 1207, 127785.	3.6	3

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253	Anion Recognition by Neutral Chalcogen Bonding Receptors: Experimental and Theoretical Investigations. <i>Chemistry - A European Journal</i> , 2020, 26, 4706-4713.	3.3	49
254	Iridium(III) coordination of N(6) modified adenine derivatives with aminoacid chains. <i>Journal of Inorganic Biochemistry</i> , 2020, 205, 111000.	3.5	7
255	Charge-Assisted Chalcogen Bonds: CSD and DFT Analyses and Biological Implication in Glucosidase Inhibitors. <i>Chemistry - A European Journal</i> , 2020, 26, 4599-4606.	3.3	42
256	Recurrent Supramolecular Motifs in a Series of Acid-Base Adducts Based on Pyridine-2,5-Dicarboxylic Acid N-Oxide and Organic Bases: Inter- and Intramolecular Hydrogen Bonding. <i>Crystal Growth and Design</i> , 2020, 20, 1738-1751.	3.0	27
257	New metal chelate constructed from Ni(NCS) ₂ and 1,2-diphenyl-1,2-bis((phenyl(pyridin-2-yl)methylene)hydrazono)ethane. <i>Inorganica Chimica Acta</i> , 2020, 509, 119707.	2.4	7
258	Toward N,P-Doped π -Extended PAHs: A One-Pot Synthesis to Diannulated 1,4,2-Diazaphospholium Triflate Salts. <i>Journal of Organic Chemistry</i> , 2020, 85, 14420-14434.	3.2	3
259	Anion-Cation Recognition Pattern, Thermal Stability and DFT-Calculations in the Crystal Structure of H ₂ dap[Cd(HEDTA)(H ₂ O)] Salt (H ₂ dap = H ₂ (N ₃ ,N ₇)-2,6-Diaminopurinium Cation). <i>Crystals</i> , 2020, 10, 304.	2.2	4
260	Anion Recognition by Neutral Chalcogen Bonding Receptors: Experimental and Theoretical Investigation. <i>Chemistry - A European Journal</i> , 2020, 26, 4644-4644.	3.3	1
261	Biological promiscuity of a binuclear Cu(II) complex of aminoguanidine Schiff base: DNA binding, anticancer activity and histidine sensing ability of the complex. <i>New Journal of Chemistry</i> , 2020, 44, 7319-7328.	2.8	21
262	Straightforward Three-Component Synthesis of N ⁺ ,N ⁺ -Disubstituted N-Alkyl-1,3,5-Triazinanes. <i>Synlett</i> , 2020, 31, 1067-1072.	1.8	7
263	9-Ethyladenine: Mechanochemical Synthesis, Characterization, and DFT Calculations of Novel Cocrystals and Salts. <i>Crystal Growth and Design</i> , 2020, 20, 2985-2997.	3.0	8
264	Relevant π -hole tetrel bonding interactions in ethyl 2-triazolyl-2-oxoacetate derivatives: Hirshfeld surface analysis and DFT calculations. <i>CrystEngComm</i> , 2020, 22, 3567-3578.	2.6	15
265	On the importance of π -hole spodium bonding in tricoordinated Hg(II) complexes. <i>Dalton Transactions</i> , 2020, 49, 17547-17551.	3.3	25
266	Diaryliodonium as a double π -hole donor: the dichotomy of thiocyanate halogen bonding provides divergent solid state arylation by diaryliodonium cations. <i>Organic Chemistry Frontiers</i> , 2020, 7, 2230-2242.	4.5	44
267	A New phenoxido/trifluoroacetato bridged heterometallic NiII ₂ CuII derivative: Structure, EPR interpretation and DFT computation. <i>Journal of Molecular Structure</i> , 2019, 1175, 948-955.	3.6	2
268	Intramolecular π -hole interactions with nitro aromatics. <i>CrystEngComm</i> , 2019, 21, 5410-5417.	2.6	16
269	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. <i>Crystal Growth and Design</i> , 2019, 19, 5819-5828.	3.0	19
270	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. <i>RSC Advances</i> , 2019, 9, 25382-25404.	3.6	15

#	ARTICLE	IF	CITATIONS
271	Antiproliferative evaluation and supramolecular association in Mn(II) and Zn(II) bipyridine complexes: Combined experimental and theoretical studies. <i>Journal of Inorganic Biochemistry</i> , 2019, 200, 110803.	3.5	37
272	5,5- π^2 -Dibenzoimidazole as building block for a new 3D Co(II) coordination polymer: A combined EPR and DFT study using UB3LYP model. <i>Polyhedron</i> , 2019, 171, 473-479.	2.2	0
273	Influence of the aromatic surface on the capacity of adsorption of VOCs by magnetite supported organic-inorganic hybrids. <i>RSC Advances</i> , 2019, 9, 24184-24191.	3.6	10
274	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. <i>Journal of Molecular Structure</i> , 2019, 1197, 458-470.	3.6	15
275	Nitropyridine-1-Oxides as Excellent π -Hole Donors: Interplay between π -Hole (Halogen, Hydrogen, Trel,) Tj ETQq1 1 0.784314 rgBT /Ov 20, 3440.	4.1	19
276	Anion- π Interactions in Light-Induced Reactions: Role in the Amidation of (Hetero)aromatic Systems with Activated π -Aryloxyamides. <i>Chemistry - A European Journal</i> , 2019, 25, 11785-11790.	3.3	38
277	Supramolecular Assemblies in Pb(II) Complexes with Hydrazido-Based Ligands. <i>Crystals</i> , 2019, 9, 323.	2.2	15
278	Exploiting 1,4-naphthoquinone and 3-iodo-1,4-naphthoquinone motifs as anion binding sites by hydrogen or halogen-bonding interactions. <i>Dalton Transactions</i> , 2019, 48, 11813-11821.	3.3	4
279	Antiproliferative evaluation and supramolecular association involving electrostatically enhanced π - π interaction in isostructural coordination solids of Mn(II), Co(II) and Zn(II) chlorobenzoates: Experimental and theoretical studies. <i>Inorganica Chimica Acta</i> , 2019, 498, 119161.	2.4	15
280	Indirect influence of alkyl substituent on sigma-hole interactions: The case study of antimony(III) diphenyldithiophosphates with covalent Sb-S and non-covalent Sb \cdots S pnictogen bonds. <i>Polyhedron</i> , 2019, 173, 114126.	2.2	18
281	π -Hole Interactions Involving Nitro Aromatic Ligands in Protein Structures. <i>Chemistry - A European Journal</i> , 2019, 25, 13436-13443.	3.3	34
282	Magnetic, luminescence, topological and theoretical studies of structurally diverse supramolecular lanthanide coordination polymers with flexible glutaric acid as a linker. <i>New Journal of Chemistry</i> , 2019, 43, 14546-14564.	2.8	29
283	π -Carboranes as dual CH \cdots π and BH \cdots π donors: theoretical study and biological significance. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19944-19950.	2.8	13
284	Supramolecular association involving antiparallel CO \cdots CO and anion- π contacts in Co(II) and Mn(II) complexes involving 2,5-pyridinedicarboxylate: Anticancer evaluation and theoretical studies. <i>Inorganica Chimica Acta</i> , 2019, 498, 119108.	2.4	17
285	Importance of π -Interactions Involving Chelate Rings in Addition to the Tetrel Bonds in Crystal Engineering: A Combined Experimental and Theoretical Study on a Series of Hemi- and Holodirected Nickel(II)/Lead(II) Complexes. <i>Crystal Growth and Design</i> , 2019, 19, 5869-5881.	3.0	53
286	Surface Modification of Pseudoboehmite-Coated Aluminum Plates with Squaramic Acid Amphiphiles. <i>ACS Omega</i> , 2019, 4, 14868-14874.	3.5	3
287	Solid-state supramolecular architectures of a series of Hg(μ) halide coordination compounds based on hydroxyl-substituted Schiff base ligands. <i>CrystEngComm</i> , 2019, 21, 6301-6312.	2.6	9
288	Supramolecular association in Cu(II) coordination complexes involving energetically significant NO \cdots NO π -hole interaction and cooperative π -stacked ternary assembly: Experimental and theoretical studies. <i>Inorganica Chimica Acta</i> , 2019, 488, 159-169.	2.4	33

#	ARTICLE	IF	CITATIONS
289	Werner type clathrates involving guest benzoic acid and benzoate in discrete Mn(II) hosts: Experimental and theoretical studies. <i>Polyhedron</i> , 2019, 159, 387-399.	2.2	28
290	Tetrel bonding interactions at work: Impact on tin and lead coordination compounds. <i>Coordination Chemistry Reviews</i> , 2019, 384, 107-125.	18.8	148
291	Halogen bonding effects on the outcome of reactions at metal centres. <i>Chemical Communications</i> , 2019, 55, 2380-2383.	4.1	23
292	Hydrogen Bond versus Halogen Bond in HXOn (X = F, Cl, Br, and I) Complexes with Lewis Bases. <i>Inorganics</i> , 2019, 7, 9.	2.7	12
293	H-Bonded anion-anion complexes in fentanyl citrate polymorphs and solvates. <i>Chemical Communications</i> , 2019, 55, 115-118.	4.1	26
294	Modulation of coordination in pincer-type isonicotinothiohydrazone Schiff base ligands by proton transfer. <i>CrystEngComm</i> , 2019, 21, 108-117.	2.6	34
295	Solvent-driven structural topology involving energetically significant intra- and intermolecular chelate ring contacts and anticancer activities of Cu(II) phenanthroline complexes involving benzoates: experimental and theoretical studies. <i>RSC Advances</i> , 2019, 9, 16339-16356.	3.6	47
296	Crystal structures of N6-modified-amino acid related nucleobase analogs (II): hybrid adenine- β -alanine and adenine-GABA molecules. <i>New Journal of Chemistry</i> , 2019, 43, 9680-9688.	2.8	13
297	π -Like-tetrel bonding interactions between Sn centres: a combined <i>ab initio</i> and CSD study. <i>Dalton Transactions</i> , 2019, 48, 11208-11216.	3.3	18
298	Methylene spacer regulated variation in molecular and crystalline architectures of cobalt(III) complexes with reduced Schiff base ligands: a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2019, 48, 11433-11447.	3.3	21
299	Adenine as a Halogen Bond Acceptor: A Combined Experimental and DFT Study. <i>Crystals</i> , 2019, 9, 224.	2.2	16
300	Gallic Acid Dimer As a Double π -Hole Donor: Evidence from X-ray, Theoretical Calculations, and Generalization from the Cambridge Structural Database. <i>Crystal Growth and Design</i> , 2019, 19, 3989-3997.	3.0	10
301	A Series of Lanthanide-Based Metal-Organic Frameworks Derived from Furan-2,5-dicarboxylate and Glutarate: Structure-Corroborated Density Functional Theory Study, Magnetocaloric Effect, Slow Relaxation of Magnetization, and Luminescent Properties. <i>Inorganic Chemistry</i> , 2019, 58, 7760-7774.	4.0	68
302	Formation of an imidazoliumyl-substituted [(L _C) ₄ P ₄] ⁴⁺ tetracation and transition metal mediated fragmentation and insertion reaction (L _C = NHC). <i>Chemical Science</i> , 2019, 10, 6868-6875.	7.4	20
303	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. <i>Journal of Molecular Structure</i> , 2019, 1195, 733-743.	3.6	31
304	Unexpected chalcogen bonds in tetravalent sulfur compounds. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11313-11319.	2.8	41
305	Energetically favorable anti-electrostatic hydrogen bonded cationic clusters in Ni(II) 3,5-dimethylpyrazole complexes: Anticancer evaluation and theoretical studies. <i>Polyhedron</i> , 2019, 168, 113-126.	2.2	36
306	On the importance of antiparallel π - π interactions in the solid state of isatin-based hydrazides. <i>New Journal of Chemistry</i> , 2019, 43, 8122-8131.	2.8	23

#	ARTICLE	IF	CITATIONS
307	Structures, Photoresponse Properties, and Biological Activity of Dicyano-Substituted 4-Aryl-2-pyridone Derivatives. <i>ACS Omega</i> , 2019, 4, 7200-7212.	3.5	16
308	Synchronized On/Off Switching of Four Binding Sites for Water in a Molecular Solomon Link. <i>Angewandte Chemie</i> , 2019, 131, 8137-8141.	2.0	5
309	Energetically significant unconventional $\pi\cdots\pi$ contacts involving fumarate in a novel coordination polymer of Zn(II): In-vitro anticancer evaluation and theoretical studies. <i>Inorganica Chimica Acta</i> , 2019, 493, 1-13.	2.4	47
310	On the preferences of five-membered chelate rings in coordination chemistry: insights from the Cambridge Structural Database and theoretical calculations. <i>Dalton Transactions</i> , 2019, 48, 5476-5490.	3.3	78
311	From π -Functional Thiazol-2-thione Derivatives to Phosphaalkenes. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 1697-1705.	2.0	2
312	Theoretical and Crystallographic Study of Lead(IV) Tetrel Bonding Interactions. <i>Chemistry - A European Journal</i> , 2019, 25, 6007-6013.	3.3	22
313	Theoretical ab Initio Study on Cooperativity Effects between Nitro π -hole and Halogen Bonding Interactions. <i>ChemPhysChem</i> , 2019, 20, 1135-1144.	2.1	21
314	Synthesis, X-ray characterization and density functional theory studies of N^6 -benzyl- N^6 -methyladenine- $M(II)$ complexes ($M = Zn, Cd$): The prominent role of $\pi\cdots\pi$, $C\cdots H\cdots\pi$ and anion- π interactions. <i>Applied Organometallic Chemistry</i> , 2019, 33, e4906.	3.0	12
315	Spectral, electrochemical and DFT studies of a trimetallic CuII Derivative: Antimycobacterial and cytotoxic activity. <i>Inorganica Chimica Acta</i> , 2019, 490, 155-162.	2.4	6
316	An inorganic-organic hybrid supramolecular framework based on the β - $[Mo_8O_{26}]^{4-}$ cluster and cobalt complex of aspartic acid: X-ray structure and DFT study. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 469-477.	0.5	12
317	Synchronized On/Off Switching of Four Binding Sites for Water in a Molecular Solomon Link. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 8053-8057.	13.8	23
318	Tri-nuclear copper-cadmium complexes of a N_2O_2 -donor ligand with the variation of counter anions: Structural elucidation and theoretical study on inter-molecular interactions. <i>Inorganica Chimica Acta</i> , 2019, 492, 142-149.	2.4	8
319	Structures, photoresponse properties and DNA binding abilities of 4-(4-pyridinyl)-2-pyridone salts. <i>RSC Advances</i> , 2019, 9, 9663-9677.	3.6	24
320	Analysis of energies of halogen and hydrogen bonding interactions in the solid state structures of vanadyl Schiff base complexes. <i>RSC Advances</i> , 2019, 9, 4789-4796.	3.6	18
321	Diverse structural assemblies of U-shaped hydrazinyl-sulfonamides: experimental and theoretical analysis of non-covalent interactions stabilizing solid state conformations. <i>CrystEngComm</i> , 2019, 21, 1780-1793.	2.6	12
322	Synthesis and characterization of a manganese(III) schiff base complex and exploration of $Br\cdots Br$ interaction in the solid state structure of the complex. <i>Journal of Coordination Chemistry</i> , 2019, 72, 3237-3247.	2.2	3
323	Definition of the chalcogen bond (IUPAC Recommendations 2019). <i>Pure and Applied Chemistry</i> , 2019, 91, 1889-1892.	1.9	322
324	Chloranilate bridged dinuclear copper(II) complexes: <i>syn</i> vs <i>anti</i> geometry tuned by the steric factor and supramolecular interactions. <i>CrystEngComm</i> , 2019, 21, 6886-6893.	2.6	9

#	ARTICLE	IF	CITATIONS
325	Formation of a tetranuclear supramolecule <i>via</i> non-covalent Pb ^{II} -Cl tetrel bonding interaction in a hemidirected lead(II) complex with a nickel(II) containing metaloligand. <i>CrystEngComm</i> , 2019, 21, 6859-6868.	2.6	30
326	Diethylaminophenyl-based Schiff base Cu(II) and V(IV) complexes: experimental and theoretical studies and cytotoxicity assays. <i>New Journal of Chemistry</i> , 2019, 43, 18832-18842.	2.8	22
327	Photosensitive Schottky barrier diode behavior of a semiconducting Co(III)-Na complex with a compartmental Schiff base ligand. <i>RSC Advances</i> , 2019, 9, 34710-34719.	3.6	19
328	Stabilization of two conformers <i>via</i> intra- or inter-molecular hydrogen bonds in a dinuclear vanadium(V) complex with a pendant Schiff base: theoretical insight. <i>RSC Advances</i> , 2019, 9, 35165-35175.	3.6	19
329	Controlled scrambling reactions to polyphosphanes <i>via</i> bond metathesis reactions. <i>Chemical Science</i> , 2019, 10, 11054-11063.	7.4	10
330	Synthesis, structure, physicochemical characterization and theoretical evaluation of non-covalent interaction energy of a polymeric copper(II)-hydrazone complex. <i>Inorganica Chimica Acta</i> , 2019, 484, 95-103.	2.4	11
331	Supramolecular association in Cu(II) and Co(II) coordination complexes of 3,5-dimethylpyrazole: Experimental and theoretical studies. <i>Inorganica Chimica Acta</i> , 2019, 484, 133-141.	2.4	36
332	A novel oxalato bridged supramolecular ternary complex of Cu(II) involving energetically significant π -hole interaction: Experimental and theoretical studies. <i>Inorganica Chimica Acta</i> , 2019, 487, 354-361.	2.4	37
333	EPR, DFT and electrochemical interpretation of a Cu(II) derivative incorporating a Schiff base precursor. <i>Polyhedron</i> , 2019, 159, 323-329.	2.2	6
334	Observation of an anion-anion interaction in a square planar copper(II) Schiff base complex: DFT study and CSD analysis. <i>Inorganica Chimica Acta</i> , 2019, 487, 465-472.	2.4	11
335	Tetranuclear Mn ^{II} /Zn ^{II} and Novel Azido-Bridged Chair-Shaped Heptanuclear Cd ^{II} Compounds: The Effect of Metal Ion and Coordination Mode of the Azide Group on the Structure of the Products. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 262-270.	2.0	15
336	Supramolecular association involving nitrile-nitrile interactions in polymeric Mn(II) coordination complexes: A combined experimental and theoretical study. <i>Inorganica Chimica Acta</i> , 2019, 487, 424-432.	2.4	30
337	A triple alkoxo bridged dinuclear cobalt(III) complex mimicking phosphatase and showing ability to degrade organic dye contaminants by photocatalysis. <i>Journal of Organometallic Chemistry</i> , 2019, 883, 52-64.	1.8	13
338	2,5-Furandicarboxylic acid as a linker for lanthanide coordination polymers: the role of heteroaromatic π - π stacking and hydrogen bonding. <i>New Journal of Chemistry</i> , 2019, 43, 2179-2195.	2.8	41
339	Synthesis, characterization and DFT study on two copper(II) complexes with a naphthalene-based Schiff base: Examples of stronger chelate-chelate interactions than those reported for classical π - π complexes. <i>Polyhedron</i> , 2019, 157, 487-494.	2.2	11
340	DFT prediction of band gap in organic-inorganic metal halide perovskites: An exchange-correlation functional benchmark study. <i>Chemical Physics</i> , 2019, 516, 225-231.	1.9	62
341	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. <i>Inorganica Chimica Acta</i> , 2019, 484, 264-275.	2.4	15
342	The role of π - π stacking and hydrogen-bonding interactions in the assembly of a series of isostructural group IIB coordination compounds. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 178-188.	0.5	13

#	ARTICLE	IF	CITATIONS
343	Anion- π Catalysis. RSC Catalysis Series, 2019, , 122-136.	0.1	0
344	Anion- π Interactions in Hollow Crystals of a Copper(II)-Cyamelurate Coordination Complex. Crystal Growth and Design, 2018, 18, 2636-2644.	3.0	12
345	Syntheses of four new asymmetric Schiff bases and their Cu(II) complexes: Theoretical calculations to rationalize the packing of molecules in the crystals. Inorganica Chimica Acta, 2018, 477, 89-101.	2.4	17
346	Non-covalent tetrel bonding interactions in hemidirectional lead(Pb^{II}) complexes with nickel(Ni^{II})-salen type metalloligands. New Journal of Chemistry, 2018, 42, 6062-6076.	2.8	44
347	Regio- π bonds: An Unexplored Link between Noble Metal Nanoparticles and Aromatic Surfaces. Chemistry - A European Journal, 2018, 24, 7228-7234.	3.3	81
348	Pb-X (X = N, S, I) tetrel bonding interactions in Pb(Pb^{II}) complexes: X-ray characterization, Hirshfeld surfaces and DFT calculations. CrystEngComm, 2018, 20, 2812-2821.	2.6	63
349	Copper(II) polyamine chelates as efficient receptors for acyclovir: syntheses, crystal structures and dft study. Polyhedron, 2018, 145, 218-226.	2.2	7
350	Formation of a water-mediated assembly of two neutral copper(Cu^{II}) Schiff base fragments with a $\text{Cu}_2(\text{NCS})_4$ moiety: exploration of non-covalent C-H \cdots H (bimetallo ring) interactions. CrystEngComm, 2018, 20, 1679-1689.	2.6	28
351	Methylene spacer regulated variation in conformation of tetradentate N_2O_2 donor Schiff bases trapped in manganese(Mn^{II}) complexes. CrystEngComm, 2018, 20, 1077-1086.	2.6	27
352	Synthesis, Substitution, and Oxidation of Imidazole-2-thione Based Tricyclic 1,4-dihydro-1,4-diphosphinines. European Journal of Inorganic Chemistry, 2018, 2018, 904-916.	2.0	11
353	Screening polymorphism in a Ni(Ni^{II}) metal-organic framework: experimental observations, Hirshfeld surface analyses and DFT studies. CrystEngComm, 2018, 20, 746-754.	2.6	68
354	Recurrent supramolecular motifs in discrete complexes and coordination polymers based on mercury halides: prevalence of chelate ring stacking and substituent effects. CrystEngComm, 2018, 20, 1065-1076.	2.6	39
355	Synergistic Anion- π Catalysis on π -Stacked Foldamers. Journal of the American Chemical Society, 2018, 140, 4884-4892.	13.7	78
356	Two Zinc(II)-Based Metal Complexes of New Pyrimidine Derived Ligand: Anion-Dependent Structural Variations and Charge Transport Property Analysis. Journal of Physical Chemistry C, 2018, 122, 8724-8734.	3.1	30
357	Mixed-ligand complexes of zinc(II) with 1,1-dicyanoethylene-2,2-dithiolate and N-donor ligands: A combined experimental and theoretical study. Journal of Molecular Structure, 2018, 1164, 334-343.	3.6	15
358	Molecular electrostatic potential and atoms-in-molecules analyses of the interplay between C-H \cdots O and lone pair-X \cdots H/metal-A interactions. Journal of Computational Chemistry, 2018, 39, 458-463.	3.3	23
359	Anion-reliant structural versatility of novel cadmium(II) complexes: Synthesis, crystal structures, photoluminescence properties and exploration of unusual O-A-S chalcogen bonding involving thiocyanate coligand. Inorganica Chimica Acta, 2018, 469, 189-196.	2.4	20
360	Estimating the energy of noncovalent interactions in a dioxovanadium(V) Schiff base complex: Exploration of its phenoxazinone synthase like activity. Polyhedron, 2018, 142, 83-92.	2.2	15

#	ARTICLE	IF	CITATIONS
361	H-Bonded anion-anion complex trapped in a squaramido-based receptor. <i>Chemical Communications</i> , 2018, 54, 1841-1844.	4.1	32
362	Valence-tautomerism-Driven Aromatic Nucleophilic Substitution in Cobalt-Bound Tetrabromocatechol Ligands Influence of Positive Charge at the Ligand Backbone on Phenoxazinone Synthase Activity. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 924-931.	2.0	18
363	Polymorphism in secondary squaramides: on the importance of π -interactions involving the four membered ring. <i>CrystEngComm</i> , 2018, 20, 237-244.	2.6	14
364	Structure guided or structure guiding? Mixed carbon/hydrogen bonding in a bis-Schiff base of <i>N</i> -allyl isatin. <i>CrystEngComm</i> , 2018, 20, 150-154.	2.6	15
365	A versatile quinoxaline derivative serves as a colorimetric sensor for strongly acidic pH. <i>Dalton Transactions</i> , 2018, 47, 17077-17085.	3.3	17
366	π -Hole halogen bonding interactions in a mixed valence cobalt(III)/cobalt(II) complex and anti-electrostatic hydrogen bonding interaction in a cobalt(III) complex: a theoretical insight. <i>CrystEngComm</i> , 2018, 20, 7281-7292.	2.6	33
367	A versatile chemosensor for the detection of Al^{3+} and picric acid (PA) in aqueous solution. <i>Dalton Transactions</i> , 2018, 47, 15907-15916.	3.3	19
368	Primary Anion π -Catalysis and Autocatalysis. <i>Journal of the American Chemical Society</i> , 2018, 140, 17867-17871.	13.7	49
369	π -Sn Tetrel Bonds in the Activation of Peroxisome Proliferator-Activated Receptors (PPARs) by Organotin Molecules. <i>Chemistry - A European Journal</i> , 2018, 24, 16582-16587.	3.3	35
370	Multicomponent Supramolecular Assemblies of Melamine and α -Hydroxycarboxylic Acids: Understanding the Hydrogen Bonding Patterns and Their Physicochemical Consequences. <i>Crystal Growth and Design</i> , 2018, 18, 6786-6800.	3.0	21
371	Bioactive Heterometallic Cu^{II} - Zn^{II} Complexes with Potential Biomedical Applications. <i>ACS Omega</i> , 2018, 3, 13343-13353.	3.5	9
372	Surface-grafted lanthanoid complexes of the tungstosilicate polyanion $[SiW_{12}O_{40}]^{4-}$: a synthetic, structural and computational investigation. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 1300-1309.	0.5	15
373	Tetrel Bonding Interactions in Perchlorinated Cyclopenta- and Cyclohexatetrelenes: A Combined DFT and CSD Study. <i>Molecules</i> , 2018, 23, 1770.	3.8	11
374	Frontispiece: Adsorption and Quantification of Volatile Organic Compounds (VOCs) by using Hybrid Magnetic Nanoparticles. <i>Chemistry - A European Journal</i> , 2018, 24, .	3.3	0
375	Effect of temperature and ligand protonation on the electronic ground state in Cu^{II} polymers having unusual secondary interactions: a magnetic and catechol oxidase study. <i>Dalton Transactions</i> , 2018, 47, 16102-16118.	3.3	11
376	Ni-Catalysed Intramolecular [4+4]-cycloadditions of bis-dienes towards eight-membered fused bicyclic systems: a combined experimental and computational study. <i>Catalysis Science and Technology</i> , 2018, 8, 5251-5258.	4.1	3
377	Joining of trinuclear $(CuL)_2M$ ($M = Mn^{II}$ and Cd^{II}) nodes by 1,3- and 1,4-benzenedicarboxylate linkers: positional isomeric effect on co-crystallization. <i>CrystEngComm</i> , 2018, 20, 6490-6501.	2.6	19
378	$Cu(II)$ - N_6 -Alkyladenine Complexes: Synthesis, X-ray Characterization and Magnetic Properties. <i>Magnetochemistry</i> , 2018, 4, 24.	2.4	2

#	ARTICLE	IF	CITATIONS
379	Intramolecular Noncovalent Carbon Bonding Interaction Stabilizes the <i>cis</i> Conformation in Acylhydrazones. <i>ChemPlusChem</i> , 2018, 83, 881-885.	2.8	19
380	Boron triel bonding: a weak electrostatic interaction lacking electron-density descriptors. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 24192-24200.	2.8	40
381	Synthesis, structures, and investigation of noncovalent interactions of 1,3-dimethyl-5-(4- <i>E</i> -pyridylazo)-6-aminouracil and their Ni(II) complexes. <i>Journal of Molecular Structure</i> , 2018, 1170, 70-81.	3.6	6
382	Synthesis, structural features, antibacterial behaviour and theoretical investigation of two new manganese(III) Schiff base complexes. <i>Polyhedron</i> , 2018, 151, 407-416.	2.2	6
383	Remote Control of Anion-Catalysis on Fullerene-Centered Catalytic Triads. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 10883-10887.	13.8	44
384	Remote Control of Anion-Catalysis on Fullerene-Centered Catalytic Triads. <i>Angewandte Chemie</i> , 2018, 130, 11049-11053.	2.0	30
385	Lone pair vs. σ -hole interactions in bromine head-containing oxalix[2]arene[2]triazines. <i>CrystEngComm</i> , 2018, 20, 3251-3257.	2.6	20
386	Zinc(ii) complexes with uncommon amina and hemiaminal ether derivatives: synthesis, structure, phosphatase activity and theoretical rationalization of ligand and complex formation. <i>New Journal of Chemistry</i> , 2018, 42, 12998-13009.	2.8	5
387	Hydrogen bonding versus π -interactions: their key competition in sildenafil solvates. <i>CrystEngComm</i> , 2018, 20, 4526-4530.	2.6	9
388	Experimental and computational investigations of the photosensitive Schottky barrier diode property of an azobenzene based small organic molecule. <i>New Journal of Chemistry</i> , 2018, 42, 13430-13441.	2.8	8
389	Nickel(II) based homo- vs heterometallic 1D coordination polymers derived from a novel 6-aminouracil building block: Structures, topologies, non-covalent interactions, magnetism, and antibacterial activity. <i>Inorganica Chimica Acta</i> , 2018, 482, 384-394.	2.4	10
390	On the importance of Pb-X (X = O, N, S, Br) tetrel bonding interactions in a series of tetra- and hexa-coordinated Pb(II) compounds. <i>CrystEngComm</i> , 2018, 20, 5033-5044.	2.6	41
391	A Ni(II) derivative incorporating tetradentate Schiff base precursor: Structure, spectral, electrochemical and DFT interpretation. <i>Journal of Molecular Structure</i> , 2018, 1173, 462-468.	3.6	4
392	Regium- vs Cation- Interactions in M ₂ and MCl (M = Cu, Ag and Au) Complexes with Small Aromatic Systems: An ab Initio Study. <i>Inorganics</i> , 2018, 6, 64.	2.7	31
393	Substituent Effects in Multivalent Halogen Bonding Complexes: A Combined Theoretical and Crystallographic Study. <i>Molecules</i> , 2018, 23, 18.	3.8	11
394	Chalcogen-like-like™ Interactions Involving Trisulphide and Triselenide Compounds: A Combined CSD and Ab Initio Study. <i>Molecules</i> , 2018, 23, 699.	3.8	22
395	Coordination Polymers Based on Phthalic Acid and Aminopyrazine Ligands: On the Importance of N-H... Interactions. <i>Polymers</i> , 2018, 10, 182.	4.5	17
396	Synthesis of Multinuclear Zn(II) Complexes Involving 8-Aminoquinoline-Based Schiff Base Ligand: Structural Diversity, DNA Binding Studies and Theoretical Calculations.. <i>ChemistrySelect</i> , 2018, 3, 7697-7706.	1.5	8

#	ARTICLE	IF	CITATIONS
397	A family of [Cu ₂], [Cu ₄] and [Cu ₅] aggregates: alteration of reaction conditions, ancillary bridges and capping anions. <i>New Journal of Chemistry</i> , 2018, 42, 14349-14364.	2.8	8
398	Crystal structures of <i>N</i> - ⁶ -modified-aminoacid/peptide nucleobase analogs: hybrid adenine-glycine and adenine-glycylglycine molecules. <i>New Journal of Chemistry</i> , 2018, 42, 14742-14750.	2.8	9
399	Adsorption and Quantification of Volatile Organic Compounds (VOCs) by using Hybrid Magnetic Nanoparticles. <i>Chemistry - A European Journal</i> , 2018, 24, 12820-12826.	3.3	14
400	Quantifying conventional π - π (aryl) and unconventional π - π (chelate) interactions in dinuclear Cu(ⁱⁱ) complexes: experimental observations, Hirshfeld surface and theoretical DFT study. <i>New Journal of Chemistry</i> , 2018, 42, 10202-10213.	2.8	72
401	Enhanced Photosensitive Schottky Diode Behavior of Pyrazine over 2-Aminopyrimidine Ligand in Copper(II)-Phthalate MOFs: Experimental and Theoretical Rationalization. <i>ACS Omega</i> , 2018, 3, 9160-9171.	3.5	26
402	A Strategy to Synthesize Molecular Knots and Links Using the Hydrophobic Effect. <i>Journal of the American Chemical Society</i> , 2018, 140, 12442-12450.	13.7	75
403	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. <i>Dalton Transactions</i> , 2018, 47, 12318-12336.	3.3	54
404	One pot synthesis of two cobalt(ⁱⁱⁱ) Schiff base complexes with chelating pyridyltetrazolate and exploration of their bio-relevant catalytic activities. <i>RSC Advances</i> , 2018, 8, 28216-28237.	3.6	29
405	Bipolar behaviour of salt-bridges: a combined theoretical and crystallographic study. <i>New Journal of Chemistry</i> , 2018, 42, 12134-12142.	2.8	18
406	A comparative experimental and theoretical investigation of hydrogen-bond, halogen-bond and π - π interactions in the solid-state supramolecular assembly of 2- and 4-formylphenyl arylsulfonates. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 816-829.	0.5	12
407	CHAPTER 9. Quantitative Analysis of Weak Non-covalent π -Hole and π -Hole Interactions. <i>Monographs in Supramolecular Chemistry</i> , 2018, , 285-333.	0.2	4
408	Heteronuclear cobalt(ⁱⁱⁱ)/sodium complexes with salen type compartmental Schiff base ligands: methylene spacer regulated variation in nuclearity. <i>Dalton Transactions</i> , 2018, 47, 331-347.	3.3	61
409	Pseudohalides regulated diverse helicity in copper(II) coordination polymers derived from a bis(aminoethoxy) ligand. <i>Polyhedron</i> , 2017, 124, 262-274.	2.2	3
410	A Ni-based MOF for selective detection and removal of Hg ²⁺ in aqueous medium: a facile strategy. <i>Dalton Transactions</i> , 2017, 46, 1943-1950.	3.3	106
411	Melamine-mediated self-assembly of a Cu(II)-methylmalonate complex assisted by π - π and anti-electrostatic H-bonding interactions. <i>Journal of Coordination Chemistry</i> , 2017, 70, 463-474.	2.2	10
412	NO ₃ ⁻ anions can act as Lewis acid in the solid state. <i>Nature Communications</i> , 2017, 8, 14522.	12.8	72
413	Carbodiphosphorane mediated synthesis of a triflyloxyphosphonium dication and its reactivity towards nucleophiles. <i>Chemical Communications</i> , 2017, 53, 2954-2957.	4.1	17
414	Introducing Supramolecular Interactions into Robust Bis(tetrabromocatecholate) Chelated Manganese(III) Systems and Biomimetic Catalytic Activity. <i>ChemistrySelect</i> , 2017, 2, 2094-2105.	1.5	9

#	ARTICLE	IF	CITATIONS
415	Synthesis and crystal structures of three new lead(II) isonicotinoylhydrazone derivatives: Anion controlled nuclearity and dimensionality. <i>Inorganica Chimica Acta</i> , 2017, 461, 192-205.	2.4	40
416	Magneto-structural and theoretical study of the weak interactions in a Mn(II) complex with a very unusual N,O-chelating coordination mode of 2-aminoterephthalate. <i>Inorganica Chimica Acta</i> , 2017, 461, 183-191.	2.4	3
417	Competition between lone pair- π , halogen- π and triel bonding interactions involving BX ₃ (X = F, Cl, Br) Tj ETQq1 1.4 0.784314 rgBT /	1.4	34
418	Design of end-on cyanato bridged trinuclear Cu(II) Schiff base complex with salen type Schiff base ligand: synthesis, structural investigation and DFT study. <i>Journal of Coordination Chemistry</i> , 2017, 70, 1389-1405.	2.2	20
419	Chelate ring stacking interactions in the supramolecular assemblies of Zn(II) and Cd(II) coordination compounds: a combined experimental and theoretical study. <i>CrystEngComm</i> , 2017, 19, 1389-1399.	2.6	36
420	Unraveling the dual character of sulfur atoms in a series of Hg(II) coordination polymers containing bis(4-pyridyl)disulfide. <i>CrystEngComm</i> , 2017, 19, 1974-1981.	2.6	11
421	On the Importance of π -Hole Beryllium Bonds: Theoretical Study and Biological Implications. <i>Chemistry - A European Journal</i> , 2017, 23, 5375-5380.	3.3	19
422	A highly selective $\text{ON}^{\ominus}\text{OFF}^{\oplus}$ -probe for colorimetric and fluorometric sensing of Cu^{2+} in water. <i>RSC Advances</i> , 2017, 7, 11312-11321.	3.6	23
423	Dangling and Hydrolyzed Ligand Arms in [Mn ₃] and [Mn ₆] Coordination Assemblies: Synthesis, Characterization, and Functional Activity. <i>Inorganic Chemistry</i> , 2017, 56, 2639-2652.	4.0	18
424	Molecular and crystalline architectures based on HgI ₂ : from metallamacrocycles to coordination polymers. <i>CrystEngComm</i> , 2017, 19, 3322-3330.	2.6	12
425	Selective and Reversible Fluoride Complexation from Water by a Cyclic Tri(phosphonio)methanide Dication. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 7907-7911.	13.8	12
426	A combined crystallographic and theoretical study of weak intermolecular interactions in crystalline squaric acid esters and amides. <i>CrystEngComm</i> , 2017, 19, 3071-3077.	2.6	9
427	Isolation of Azadiphosphiridines and Diphosphenimines by Cycloaddition of Azides and a Cationic Diphosphene. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 6218-6222.	13.8	14
428	Selective and Reversible Fluoride Complexation from Water by a Cyclic Tri(phosphonio)methanide Dication. <i>Angewandte Chemie</i> , 2017, 129, 8015-8019.	2.0	2
429	A survey of the different roles of polyoxometalates in their interaction with amino acids, peptides and proteins. <i>Dalton Transactions</i> , 2017, 46, 6812-6829.	3.3	116
430	Supramolecular nanotubes based on halogen bonding interactions: cooperativity and interaction with small guests. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12936-12941.	2.8	26
431	The Mouse in a Trap: Observation of a C(sp ³)- π -C(sp ³) Interaction in a Discrete CFC Pair by the Crystal Sponge Method. <i>Crystal Growth and Design</i> , 2017, 17, 3611-3615.	3.0	13
432	Supramolecular coordination polymers of La(III), Ce(III), Sm(III), Gd(III) and Eu(III) decorated with rigid 5-hydroxy-1,3-benzenedicarboxylate and flexible hexane-1,6-dicarboxylate linkers: Syntheses, structures, DFT study, luminescence and magnetic properties. <i>Polyhedron</i> , 2017, 134, 153-165.	2.2	5

#	ARTICLE	IF	CITATIONS
433	Importance of C-H...H interactions in stabilizing the syn/anti arrangement of pendant alkoxy side arms in two manganese(IV) Schiff base complexes: exploration of catechol oxidase and phenoxazinone synthase like activities. <i>New Journal of Chemistry</i> , 2017, 41, 8053-8065.	2.8	16
434	The roles of H-bonding, π -stacking, and antiparallel CO π -CO interactions in the formation of a new Gd(III) coordination polymer based on pyridine-2,6-dicarboxylic acid. <i>Inorganic Chemistry Communication</i> , 2017, 83, 24-26.	3.9	9
435	A trigonal prismatic anionic iron(III) complex of a radical o-aminobenzosemiquinonate derivative: structural and spectral analyses. <i>New Journal of Chemistry</i> , 2017, 41, 7283-7291.	2.8	6
436	On the Importance of Nonbonding Donor-Acceptor Interactions Involving PO ₂ Radicals: An ab Initio Study. <i>ChemPhysChem</i> , 2017, 18, 2191-2196.	2.1	1
437	Synthesis and structure of 1,3-dimethyl-5-(p-sulfonamide-phenylazo)-6-aminouracil and its Ni(II) complex: Topological insights and investigation for noncovalent interactions. <i>Journal of Molecular Structure</i> , 2017, 1141, 225-236.	3.6	12
438	Synthesis, Characterization, DFT Study, Catechol Oxidase and Phenoxazinone Synthase Like Activities of Two New Manganese(IV) Schiff Base Complexes. <i>ChemistrySelect</i> , 2017, 2, 2975-2984.	1.5	18
439	Unveiling the effects of the in situ generated arene anion radical and imine radical on catecholase like activity: a DFT supported experimental investigation. <i>Dalton Transactions</i> , 2017, 46, 5888-5900.	3.3	24
440	Mononuclear and dinuclear trimethylplatinum(IV) iodide complexes of 3-substituted pyridines. <i>New Journal of Chemistry</i> , 2017, 41, 3498-3507.	2.8	5
441	π -hole interactions at work: crystal engineering with nitro-derivatives. <i>CrystEngComm</i> , 2017, 19, 1933-1937.	2.6	63
442	Estimation of conventional C-H... π (arene), unconventional C-H... π (chelate) and C-H... π (thiocyanate) interactions in hetero-nuclear nickel-cadmium complexes with a compartmental Schiff base. <i>Dalton Transactions</i> , 2017, 46, 5384-5397.	3.3	60
443	Synthesis and supramolecular self-assembly of thioxothiazolidinone derivatives driven by H-bonding and diverse π -hole interactions: A combined experimental and theoretical analysis. <i>Journal of Molecular Structure</i> , 2017, 1139, 209-221.	3.6	11
444	Ambiguous reactivity of Li/Cl phosphinidenoid complexes under redox conditions - a novel dichotomy in phosphorus chemistry. <i>Chemical Communications</i> , 2017, 53, 933-936.	4.1	3
445	EPR interpretation, magnetism and biological study of a Cu(II) dinuclear complex assisted by a schiff base precursor. <i>Journal of Biological Inorganic Chemistry</i> , 2017, 22, 481-495.	2.6	14
446	X-ray Crystal Structure of a Metalled Double-Helix Generated by Infinite and Consecutive C*Ag ⁺ (C*:N ¹ -Hexylcytosine) Base Pairs through Argentophilic and Hydrogen Bond Interactions. <i>Chemistry - A European Journal</i> , 2017, 23, 2103-2108.	3.3	41
447	Solid-state inclusion of C ₆₀ and C ₇₀ in a co-polymer induced by metal-ligand coordination of a Zn-porphyrin cage with a bis-pyridyl perylene derivative. <i>CrystEngComm</i> , 2017, 19, 4911-4919.	2.6	14
448	Observation of π -hole interactions in the solid state structures of three new copper(II) complexes with a tetradentate N ₄ donor Schiff base: Exploration of their cytotoxicity against MDA-MB 468 cells. <i>Polyhedron</i> , 2017, 123, 334-343.	2.2	41
449	Concurrent aerogen bonding and lone pair/anion- π interactions in the stability of organoxenon derivatives: a combined CSD and ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30063-30068.	2.8	30
450	Cooperative influence of pseudohalides and ligand backbone of Schiff-bases on nuclearity and stereochemistry of cobalt(III) complexes: experimental and theoretical investigation. <i>Dalton Transactions</i> , 2017, 46, 15257-15268.	3.3	23

#	ARTICLE	IF	CITATIONS
451	Donor-acceptor interactions in tri(phosphonio)methanide dications [(Ph ₃ P) ₂ CP(X)Ph ₂] ₂ ⁺ (X = H, Me). <i>Talanta</i> , 2017, 168, 1078-1084.	3.3	14
452	A Combined Experimental and Theoretical Study on the Formation of a Cyclic Tetrameric Water Cluster and a Similar Type of Cyclic Cluster in Copper(II) Schiff Base Complexes. <i>ChemistrySelect</i> , 2017, 2, 9336-9343.	1.5	34
453	Theoretical investigation on molecular structure of a new mononuclear copper(II) thiocyanato complex with tridentate Schiff base ligand. <i>Journal of Coordination Chemistry</i> , 2017, 70, 3715-3726.	2.2	9
454	Influence of ancillary ligands on preferential geometry and biomimetic catalytic activity in manganese(III)-catecholate systems: A combined experimental and theoretical study. <i>Journal of Inorganic Biochemistry</i> , 2017, 176, 77-89.	3.5	9
455	A polynuclear and two dinuclear copper(II) Schiff base complexes: Synthesis, characterization, self-assembly, magnetic property and DFT study. <i>Polyhedron</i> , 2017, 137, 332-346.	2.2	21
456	Nuclearity versus oxidation state in the catalytic efficiency of Mn(II)/Mn(III) azo Schiff base complexes: computational study on supramolecular interactions and phenoxazinone synthase-like activity. <i>New Journal of Chemistry</i> , 2017, 41, 11607-11618.	2.8	10
457	The development of a promising photosensitive Schottky barrier diode using a novel Cd(II)-based coordination polymer. <i>Dalton Transactions</i> , 2017, 46, 13531-13543.	3.3	49
458	The first X-ray structure of a silver-nucleotide complex: interaction of ion Ag(I) with cytidine-5'-monophosphate. <i>CrystEngComm</i> , 2017, 19, 5830-5834.	2.6	18
459	Both end-on and end-to-end azide bridged tetranuclear ferromagnetic nickel(II) Schiff base complexes. <i>New Journal of Chemistry</i> , 2017, 41, 13585-13592.	2.8	11
460	Benzyl Dihydrazone versus Thiosemicarbazone Schiff Base: Effects on the Supramolecular Arrangement of Cobalt Thiocyanate Complexes and the Generation of CoN ₆ and CoN ₄ S ₂ Coordination Spheres. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 4763-4772.	2.0	54
461	Anion Catalysis on Fullerenes. <i>Journal of the American Chemical Society</i> , 2017, 139, 13296-13299.	13.7	74
462	Suitable Interplay between Various Conventional and Unconventional Non-Covalent Interactions in Forming Self-Assembled Supramolecules of Two Ni(II)/Zn(II) Schiff Base Complexes. <i>ChemistrySelect</i> , 2017, 2, 7880-7887.	1.5	16
463	Synthetic Modulation of a Chemosensor Affords Target Metal Ion Switch from Zn ²⁺ to Al ³⁺ . <i>ChemistrySelect</i> , 2017, 2, 5414-5420.	1.5	7
464	A Cd(II)-based MOF as a photosensitive Schottky diode: experimental and theoretical studies. <i>Dalton Transactions</i> , 2017, 46, 11239-11249.	3.3	66
465	Estimation of non-covalent C-H...N (chelate ring) and hydrogen bonding interactions in vanadium(V) Schiff base complexes: Methylene spacer regulated variation in self-assembly. <i>Inorganica Chimica Acta</i> , 2017, 467, 212-220.	2.4	11
466	Phosphatase Mimicking Activity of Two Zinc(II) Schiff Base Complexes with Zn ₂ O ₂ Cores: NBO Analysis and MEP Calculation to Estimate Non-Covalent Interactions. <i>ChemistrySelect</i> , 2017, 2, 6286-6295.	1.5	30
467	Isolation of Azadiphosphiridines and Diphosphenimines by Cycloaddition of Azides and a Cationic Diphosphene. <i>Angewandte Chemie</i> , 2017, 129, 6314-6318.	2.0	2
468	Accidental Orthogonality Induced Weak Magnetic Coupling in a Dinuclear Copper(II) Complex: Exploration of Unconventional Ca-H...N...N...N(SCN) Interactions and Catechol Oxidase Activity. <i>ChemistrySelect</i> , 2017, 2, 6535-6543.	1.5	18

#	ARTICLE	IF	CITATIONS
469	A Combined Experimental and Theoretical Study to Explore the Importance of π -Hole Carbon Bonding Interactions in Stabilizing Molecular Assemblies. <i>ChemistrySelect</i> , 2017, 2, 10586-10594.	1.5	16
470	Hydrogen- and halogen-bond cooperativity in determining the crystal packing of dihalogen charge-transfer adducts: a study case from heterocyclic pentatomic chalcogenone donors. <i>CrystEngComm</i> , 2017, 19, 4401-4412.	2.6	24
471	Importance of π -CF ₃ - π -O Tetrel Bonding Interactions in Biological Systems. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5371-5376.	2.5	69
472	A Schiff base platform: structures, sensing of Zn(II) and PPI in aqueous medium and anticancer activity. <i>Dalton Transactions</i> , 2017, 46, 9498-9510.	3.3	56
473	New pyridoxal based chemosensor for selective detection of Zn ²⁺ : Application in live cell imaging and phosphatase activity response. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 334, 86-100.	3.9	17
474	Solvent dependent nuclearity of manganese complexes with a polydentate hydrazone-based ligand and thiocyanate anions. <i>Inorganica Chimica Acta</i> , 2017, 455, 204-212.	2.4	9
475	Ligand Flexibility Controlled and Solvent-Induced Nuclearity Conversion in Cu ^{II} -Based Catecholase Models: A Deep Insight Through Combined Experimental and Theoretical Investigations. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 133-145.	2.0	28
476	Fluorescent sensing of Al ³⁺ by benzophenone based Schiff base chemosensor and live cell imaging applications: Impact of keto-enol tautomerism. <i>Sensors and Actuators B: Chemical</i> , 2017, 239, 1194-1204.	7.8	48
477	The crucial role of chelate-chelate stacking interactions in the crystal structure of a square planar copper(II) complex. <i>Journal of Molecular Structure</i> , 2017, 1127, 355-360.	3.6	13
478	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. <i>Polyhedron</i> , 2017, 121, 199-205.	2.2	26
479	On the Importance of Halogen-Halogen Interactions in the Solid State of Fullerene Halides: A Combined Theoretical and Crystallographic Study. <i>Crystals</i> , 2017, 7, 191.	2.2	17
480	Crystallographic characterization and elucidation of unconventional interactions of small molecules. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, C958-C958.	0.1	0
481	RCH ₃ - π -O Interactions in Biological Systems: Are They Trifurcated H-Bonds or Noncovalent Carbon Bonds?. <i>Crystals</i> , 2016, 6, 26.	2.2	68
482	Experimental and theoretical study of weak intermolecular interactions in crystalline tertiary squaramides. <i>CrystEngComm</i> , 2016, 18, 6437-6443.	2.6	13
483	Asymmetric Hydrogenation of Seven-Membered C=N-Containing Heterocycles and Rationalization of the Enantioselectivity. <i>Chemistry - A European Journal</i> , 2016, 22, 10607-10613.	3.3	38
484	Electrostatically enhanced F \cdots F interactions through hydrogen bonding, halogen bonding and metal coordination: an ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20381-20388.	2.8	32
485	A combined experimental and theoretical study on supramolecular assemblies in octahedral cobalt(III) salicylaldehyde complexes having pendant side arms. <i>Polyhedron</i> , 2016, 112, 86-95.	2.2	15
486	Anion-dependent structural diversity of cadmium(II) complexes: synthesis, crystal structures, luminescence properties, and unusual C-H \cdots F supramolecular interactions involving π -aromatic M ₂ X ₂ cores. <i>Journal of Coordination Chemistry</i> , 2016, 69, 1188-1205.	2.2	8

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487	A combined experimental and computational study of supramolecular assemblies in two photoluminescent cadmium(II) complexes with halosalicylaldimine Schiff bases. <i>Inorganica Chimica Acta</i> , 2016, 450, 321-329.	2.4	10
488	Metal-organic and supramolecular lead(II) networks assembled from isomeric nicotinoylhydrazone blocks: the effects of ligand geometry and counter-ion on topology and supramolecular assembly. <i>CrystEngComm</i> , 2016, 18, 5375-5385.	2.6	40
489	Anion dependent supramolecular architectures in Cu(II) complexes containing N2O-donor Schiff-base and 4,4'-bipyridine ligands: Structural analyses and theoretical studies. <i>Inorganica Chimica Acta</i> , 2016, 448, 26-33.	2.4	12
490	Exploration of unconventional π -hole and C-H \cdots H-C types of supramolecular interactions in a trinuclear Cd(II) and a heteronuclear Cd(II)-Ni(II) complex and experimental evidence for preferential site selection of the ligand by 3d and 4d metal ions. <i>RSC Advances</i> , 2016, 6, 39376-39386.	3.6	13
491	Synthesis, X-ray characterization and DFT study of a novel Fe(III)-pyridine-2,6-dicarboxylic acid N-oxide complex with unusual coordination mode. <i>Inorganica Chimica Acta</i> , 2016, 449, 44-51.	2.4	16
492	Synthesis, X-ray characterization, DFT calculations and Hirshfeld surface analysis of Zn(II) and Cd(II) complexes based on isonicotinoylhydrazone ligand. <i>CrystEngComm</i> , 2016, 18, 4587-4596.	2.6	27
493	Catecholase activity, DNA binding and cytotoxicity studies of a Cu(II) complex of a pyridoxal schiff base: synthesis, X-ray crystal structure, spectroscopic, electrochemical and theoretical studies. <i>RSC Advances</i> , 2016, 6, 86851-86861.	3.6	38
494	Coordination Behavior of Chelidamic Acid With V ^V , Ni ^{II} , Fe ^{III} , and Ca ^{II} : Syntheses, X-ray Characterization and DFT Studies. <i>ChemistrySelect</i> , 2016, 1, 1556-1566.	1.5	8
495	Two Polymorphic Forms of a Six-Coordinate Mononuclear Cobalt(II) Complex with Easy-Plane Anisotropy: Structural Features, Theoretical Calculations, and Field-Induced Slow Relaxation of the Magnetization. <i>Inorganic Chemistry</i> , 2016, 55, 8502-8513.	4.0	72
496	π -Hole Interactions Involving Nitro Compounds: Directionality of Nitrate Esters. <i>Crystal Growth and Design</i> , 2016, 16, 5520-5524.	3.0	67
497	Auxiliary Part of Ligand Mediated Unique Coordination Chemistry of Copper (II). <i>ChemistrySelect</i> , 2016, 1, 615-625.	1.5	20
498	A combined experimental and computational study on supramolecular assemblies in hetero-tetranuclear nickel(II)-cadmium(II) complexes with N ₂ O ₄ -donor compartmental Schiff bases. <i>Dalton Transactions</i> , 2016, 45, 15048-15059.	3.3	46
499	Weak interactions within nitryl halide heterodimers. <i>New Journal of Chemistry</i> , 2016, 40, 9060-9072.	2.8	8
500	Carboxylate Coordination Assisted Aggregation for Quasi-Tetrahedral and Partial-Dicubane [Cu ₄] Coordination Clusters. <i>ChemistrySelect</i> , 2016, 1, 64-75.	1.5	13
501	Solvent-Triggered Cis/Trans Isomerism in Cobalt Dioxolene Chemistry: Distinguishing Effects of Packing on Valence Tautomerism. <i>Inorganic Chemistry</i> , 2016, 55, 8331-8340.	4.0	29
502	Modulation in π - π , cation- π and C-H \cdots H-C interactions varying the counter anions in square planar nickel(II) Schiff base complexes: A combined experimental and theoretical study. <i>Polyhedron</i> , 2016, 119, 451-459.	2.2	9
503	Halide Ion Mediated Aldehyde-Amine Condensation Leading to Schiff-base and Cyclized Non-Schiff-base Ligand Complexes of CdII: A Combined Experimental and Theoretical Investigation. <i>ChemistrySelect</i> , 2016, 1, 4539-4549.	1.5	1
504	Synthesis and Investigation of Solid- and Solution-State Structures of Nickel(II) Complexes with 1,3-Dimethyl-5-(aryloxy)-6-aminouracil. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 5585-5593.	2.0	10

#	ARTICLE	IF	CITATIONS
505	Self-assembly synthesis, structure, topology, and magnetic properties of a mononuclear Fe(ⁱⁱⁱ)-violurate derivative: a combined experimental and theoretical study. Dalton Transactions, 2016, 45, 16166-16172.	3.3	18
506	A combined experimental and theoretical study on two new dinuclear cadmium(II) Schiff base complexes with selenocyanate- ^p -Se. Inorganica Chimica Acta, 2016, 453, 51-61.	2.4	11
507	On the Versatility of BH ₂ X (X=F, Cl, Br, and I) Compounds as Halogen-, Hydrogen-, and Triel-Bond Donors: An Ab-Initio Study. ChemPhysChem, 2016, 17, 3181-3186.	2.1	28
508	On the Versatility of BH ₂ X (X=F, Cl, Br, and I) Compounds as Halogen-, Hydrogen-, and Triel-Bond Donors: An Ab-Initio Study. ChemPhysChem, 2016, 17, 3150-3150.	2.1	1
509	Irradiation Specified Conformational Change in a Small Organic Compound and Its Effect on Electrical Properties. Journal of Physical Chemistry C, 2016, 120, 25557-25563.	3.1	20
510	Theoretical study on σ - and π -hole carbon-carbon bonding interactions: implications in CFC chemistry. Physical Chemistry Chemical Physics, 2016, 18, 32155-32159.	2.8	22
511	Charge-assisted triel bonding interactions in solid state chemistry: A combined computational and crystallographic study. Chemical Physics Letters, 2016, 666, 73-78.	2.6	43
512	The role of unconventional stacking interactions in the supramolecular assemblies of Hg(ⁱⁱ) coordination compounds. CrystEngComm, 2016, 18, 9056-9066.	2.6	40
513	σ -Hole Opposite to a Lone Pair: Unconventional Pnictogen Bonding Interactions between ZF ₃ (Z=N, P, As, and Sb) Compounds and Several Donors. ChemPhysChem, 2016, 17, 1608-1614.	2.1	68
514	A novel method for copper(ⁱⁱ) mediated region-selective bromination of aromatic rings under mild conditions. RSC Advances, 2016, 6, 61214-61220.	3.6	20
515	Cationic 5-phosphonio-substituted N-heterocyclic carbenes. Dalton Transactions, 2016, 45, 11384-11396.	3.3	45
516	On the importance of tetrel bonding interactions in lead(ⁱⁱ) complexes with (iso)nicotinohydrazide based ligands and several anions. Dalton Transactions, 2016, 45, 10708-10716.	3.3	78
517	Fluorescent Lipid Nanoparticles as Biomembrane Models for Exploring Emerging Contaminant Bioavailability Supported by Density Functional Theory Calculations. Environmental Science & Technology, 2016, 50, 7135-7143.	10.0	9
518	Theoretical study on the degree of delocalization of unpaired spin in two mixed valence copper(II/I) complexes with isomeric chelating diamines and iodide. Inorganica Chimica Acta, 2016, 451, 16-22.	2.4	2
519	Two mixed-ligand cadmium(ⁱⁱ) compounds bearing 5-nitrosopyrimidine and N-donor aromatic blocks: self-assembly generation, structural and topological features, DFT studies, and Hirshfeld surface analysis. CrystEngComm, 2016, 18, 5647-5657.	2.6	23
520	A rare doubly nitrate and phenoxido bridged trimetallic Cu ^{II} complex: EPR, antiferromagnetic coupling and theoretical rationalization. RSC Advances, 2016, 6, 54856-54865.	3.6	9
521	On the Importance of Noncovalent Carbon-Bonding Interactions in the Stabilization of a 1D Co(II) Polymeric Chain as a Precursor of a Novel 2D Coordination Polymer. Journal of Physical Chemistry B, 2016, 120, 6803-6811.	2.6	19
522	Inorganic-organic hybrid materials based on PbBr ₂ and pyridine-hydrazone blocks: structural and theoretical study. RSC Advances, 2016, 6, 60385-60393.	3.6	24

#	ARTICLE	IF	CITATIONS
541	The Bright Future of Unconventional π - π Hole Interactions. <i>ChemPhysChem</i> , 2015, 16, 2496-2517.	2.1	569
542	Competition between Halogen Bonding and π - π Hole Interactions Involving Various Donors: The Role of Dispersion Effects. <i>ChemPhysChem</i> , 2015, 16, 3108-3113.	2.1	34
543	Supramolecularly Regulated Ligands for Asymmetric Hydroformylations and Hydrogenations. <i>Chemistry - A European Journal</i> , 2015, 21, 11417-11426.	3.3	46
544	Theoretical Study on the Dual Behavior of XeO_3 and XeF_4 toward Aromatic Rings: Lone Pair π versus Aerogen π Interactions. <i>ChemPhysChem</i> , 2015, 16, 3625-3630.	2.1	63
545	Nature of Noncovalent Carbon π -Bonding Interactions Derived from Experimental Charge ρ Density Analysis. <i>ChemPhysChem</i> , 2015, 16, 2530-2533.	2.1	57
546	Hydrogen Bond, π - π , and $\text{CH} \cdots \pi$ Interactions Governing the Supramolecular Assembly of Some Hydrazone Ligands and Their Mn^{II} Complexes π Structural and Theoretical Interpretation. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 1958-1972.	2.0	84
547	Design of Lead(II) Metal-Organic Frameworks Based on Covalent and Tetrel Bonding. <i>Chemistry - A European Journal</i> , 2015, 21, 17951-17958.	3.3	93
548	On the Importance of $\text{C} \cdots \text{H} \cdots \pi$ and $\text{C} \cdots \text{H} \cdots \pi \cdots \pi \cdots \text{H} \cdots \text{C}$ Interactions in the Solid State Structure of 15 π -Lipoxygenase Inhibitors Based on Eugenol Derivatives. <i>ChemPhysChem</i> , 2015, 16, 2260-2266.	2.1	17
549	Two types of nitrito support for μ_4 -oxido-bridged $[\text{Cu}_4]$ complexes: synthesis, crystal structures, magnetic properties and DFT analysis. <i>Dalton Transactions</i> , 2015, 44, 6107-6117.	3.3	13
550	Exploration of $\text{CH} \cdots \pi$ interactions involving the π -system of pseudohalide coligands in metal complexes of a Schiff-base ligand. <i>CrystEngComm</i> , 2015, 17, 4680-4690.	2.6	78
551	Syntheses, crystal structures and density functional theory investigations of copper(II) complexes bearing tridentate Schiff base ligands derived from 8-aminoquinoline. <i>CrystEngComm</i> , 2015, 17, 5664-5671.	2.6	12
552	Anion- π Interactions in Supramolecular Chemistry and Catalysis. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 471-500.	0.6	8
553	Enantiopure bisphosphine ligands with appended crown ether groups as regulation sites for Rh-mediated hydrogenations. <i>Tetrahedron</i> , 2015, 71, 4490-4494.	1.9	24
554	An experimental and computational investigations of supramolecular anion- π -anion assemblies in mononuclear $\text{Zn}(\text{II})$ complexes with a versatile tetradentate N-donor Schiff base ligand. <i>Polyhedron</i> , 2015, 102, 764-772.	2.2	4
555	Influence of para substituents in controlling photophysical behavior and different non-covalent weak interactions in zinc complexes of a phenol based π -end-off π -compartmental ligand. <i>Dalton Transactions</i> , 2015, 44, 20032-20044.	3.3	19
556	Importance of polarization assisted/resonance assisted hydrogen bonding interactions and unconventional interactions in crystal formations of five new complexes bearing chelidamic acid through a proton transfer mechanism. <i>RSC Advances</i> , 2015, 5, 72923-72936.	3.6	50
557	Synthesis, Structures, and DFT Study of CuBr Based Coordination Polymers via in Situ Reduction of Copper(II). <i>Crystal Growth and Design</i> , 2015, 15, 257-267.	3.0	12
558	Rationalization of Noncovalent Interactions within Six New $\text{M}^{\text{II}}/8\text{-Aminoquinoline}$ Supramolecular Complexes ($\text{M}^{\text{II}} = \text{Mn}, \text{Cu}, \text{and Cd}$): A Combined Experimental and Theoretical DFT Study. <i>Crystal Growth and Design</i> , 2015, 15, 1351-1361.	3.0	97

#	ARTICLE	IF	CITATIONS
559	Electronic Structure of N_2P_2 Four-Membered Rings and the Effect of Their Ligand Coordination to $M(CO)_5$ (Cr, Mo, and W). <i>Organometallics</i> , 2015, 34, 355-360.	2.3	10
560	Surprising behaviour of $M-CO(\text{lone pair})-\pi(\text{arene})$ interactions in the solid state of fluorinated oxaphosphirane complexes. <i>CrystEngComm</i> , 2015, 17, 1769-1772.	2.6	26
561	Cadmium(II) complexes containing N,N-dimethylviolurate as ligand or counteranion: synthesis, characterization, crystal structures and DFT study. <i>RSC Advances</i> , 2015, 5, 10826-10836.	3.6	18
562	Unprecedented structural variations in trinuclear mixed valence $Co(\text{II})/Co(\text{III})$ complexes: theoretical studies, pnictogen bonding interactions and catecholase-like activities. <i>Dalton Transactions</i> , 2015, 44, 3862-3876.	3.3	124
563	From monomers to polymers: steric and supramolecular effects on dimensionality of coordination architectures of heteroleptic mercury(II) halogenide-tetradentate Schiff base complexes. <i>CrystEngComm</i> , 2015, 17, 3493-3502.	2.6	29
564	π -Hole aerogen bonding interactions. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24748-24753.	2.8	98
565	Supramolecular interactions through lone pair(lp)- π and hydrogen bonding in cobalt(III) and manganese(II) derivatives of N,N-dimethylvioluric acid: A combined experimental and theoretical study. <i>Inorganica Chimica Acta</i> , 2015, 435, 178-186.	2.4	12
566	On the nature of $M-CO(\text{lone pair})-\pi(\text{arene})$ interactions in the solid state of fluorinated oxaphosphirane complexes. <i>CrystEngComm</i> , 2015, 17, 6736-6743.	2.6	11
567	Observation of novel oxygen \cdots oxygen interaction in supramolecular assembly of cobalt(III) Schiff base complexes: a combined experimental and computational study. <i>RSC Advances</i> , 2015, 5, 73028-73039.	3.6	36
568	Application of a novel 2D cadmium(II)-MOF in the formation of a photo-switch with a substantial on/off ratio. <i>Chemical Communications</i> , 2015, 51, 12974-12976.	4.1	93
569	The N-atom in $[N(PR_3)_2]^{2+}$ cations (R = Ph, Me) can act as electron donor for (pseudo) anti-electrostatic interactions. <i>CrystEngComm</i> , 2015, 17, 3768-3771.	2.6	17
570	Synthesis, X-ray characterization and DFT studies of N-benzimidazolyl-pyrimidine- $M(\text{II})$ complexes (M = Cu, Co and Ni): the prominent role of π -hole and anion- π interactions. <i>CrystEngComm</i> , 2015, 17, 5987-5997.	2.6	18
571	Reconciling Experiment and Theory in the Use of Aryl-Extended Calix[4]pyrrole Receptors for the Experimental Quantification of Chloride- π Interactions in Solution. <i>International Journal of Molecular Sciences</i> , 2015, 16, 8934-8948.	4.1	10
572	Experimental observation and theoretical investigation of a novel $Cd(\text{II})$ complex with π -hole interactions involving nitro groups. <i>CrystEngComm</i> , 2015, 17, 3912-3916.	2.6	26
573	A New Family of Ni_4 and Ni_6 Aggregates from the Self-Assembly of $[Ni_2]$ Building Units: Role of Carboxylate and Carbonate Bridges. <i>Inorganic Chemistry</i> , 2015, 54, 4709-4723.	4.0	46
574	Synthesis, crystal structures, magnetic properties and DFT calculations of nitrate and oxalate complexes with 3,5 dimethyl-1-(2-pyridyl)-pyrazole- $Cu(\text{II})$. <i>RSC Advances</i> , 2015, 5, 45082-45091.	3.6	8
575	Aerogen Bonding Interaction: A New Supramolecular Force?. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 7340-7343.	13.8	294
576	Hydrothermal synthesis, X-ray structure and DFT and magnetic studies of a $(H_2SiW_{12}O_{40})^{2-}$ based one-dimensional linear coordination polymer. <i>Dalton Transactions</i> , 2015, 44, 8824-8832.	3.3	34

#	ARTICLE	IF	CITATIONS
577	Two new copper and nickel complexes of pyridine-2,6-dicarboxylic acid N-oxide and their proton transferred salts: Solid state and DFT insights. <i>Inorganica Chimica Acta</i> , 2015, 438, 135-145.	2.4	16
578	Solvent-controlled construction of manganese(II) complexes with 4-acetylpyridine nicotinoylhydrazone ligand. <i>Inorganica Chimica Acta</i> , 2015, 438, 220-231.	2.4	8
579	New chloride-dimethylsulfoxide-iridium(III) complex with histaminium. <i>Polyhedron</i> , 2015, 102, 735-740.	2.2	2
580	The first mixed-ligand coordination compound involving 8-aminoquinoline and pyridine-2,6-dicarboxylate: synthesis, X-ray crystal structure, and DFT studies. <i>Journal of Coordination Chemistry</i> , 2015, 68, 3599-3610.	2.2	8
581	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. <i>Polyhedron</i> , 2015, 101, 257-269.	2.2	17
582	A crystalline sponge based on dispersive forces suitable for X-ray structure determination of included molecular guests. <i>Chemical Science</i> , 2015, 6, 5466-5472.	7.4	54
583	A new solvated complex of the uranyl ion (UO ₂ ²⁺) with 8-hydroxyquinoline. <i>Inorganica Chimica Acta</i> , 2015, 426, 136-141.	2.4	6
584	Directionality of π -holes in nitro compounds. <i>Chemical Communications</i> , 2015, 51, 1491-1493.	4.1	130
585	Synthesis, crystal structure, antimicrobial screening and density functional theory calculation of nickel(II), cobalt(II) and zinc(II) mononuclear Schiff base complexes. <i>Inorganica Chimica Acta</i> , 2015, 425, 211-220.	2.4	36
586	Synthesis, structure, solution and DFT studies of a pyrazine-bridged binuclear Cu(II) complex: On the importance of noncovalent interactions in the formation of crystalline network. <i>Journal of Molecular Structure</i> , 2015, 1079, 78-86.	3.6	5
587	Synthesis, structure and DFT study of a chelidamic acid based Cu coordination polymer: On the importance of π - π interactions and hexameric water clusters. <i>Journal of Molecular Structure</i> , 2015, 1080, 30-36.	3.6	20
588	3-Picoline Mediated Self-Assembly of M(II)-Malonate Complexes (M = Ni/Co/Mn/Mg/Zn/Cu) Assisted by Various Weak Forces Involving Lone Pair π , π - π , and Anion π -Hole Interactions. <i>Journal of Physical Chemistry B</i> , 2014, 118, 14713-14726.	2.6	81
589	Copper-Assisted Hemiacetal Synthesis: A Cu ^{II} Chain Obtained by a One-Step in situ Reaction of Picolinaldehyde. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 3271-3278.	2.0	4
590	Substituent effects in cation π interactions revisited: a general approach based on intrinsic properties of the arenes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 1322-1326.	2.8	28
591	Triple-bridged ferromagnetic nickel(ii) complexes: A combined experimental and theoretical DFT study on stabilization and magnetic coupling. <i>Dalton Transactions</i> , 2014, 43, 6455.	3.3	28
592	Analyses of supramolecular interactions present in a coordination polymer of Mn(II) with 2-picolinate and 4,4'-Azobis(pyridine). <i>Inorganic Chemistry Communication</i> , 2014, 41, 1-5.	3.9	6
593	Crystal structures and DFT calculations of new chlorido-dimethylsulfoxide-MIII (M = Ir, Ru, Rh) complexes with the N-pyrazolyl pyrimidine donor ligand: kinetic vs. thermodynamic isomers. <i>Dalton Transactions</i> , 2014, 43, 6353.	3.3	6
594	Synthesis, structural characterization, theoretical calculations and catecholase mimetic activity of manganese-Schiff base complexes. <i>Polyhedron</i> , 2014, 75, 40-49.	2.2	41

#	ARTICLE	IF	CITATIONS
595	Electronic Structure of N ₂ P ₂ Four-Membered Rings. <i>ChemPhysChem</i> , 2014, 15, 1599-1603.	2.1	3
596	Recent developments in the crystal engineering of diverse coordination modes (O ¹²) for Keggin-type polyoxometalates in hybrid inorganic-organic architectures. <i>Coordination Chemistry Reviews</i> , 2014, 275, 1-18.	18.8	159
597	On the relationship between ring strain energies and $\tilde{\sigma}$ -atoms-in-molecules TM properties in N ₂ P ₂ rings. <i>Chemical Physics Letters</i> , 2014, 597, 40-44.	2.6	7
598	Molecular Recognition of Nucleotides in Water by Scorpion-Type Receptors Based on Nucleobase Discrimination. <i>Chemistry - A European Journal</i> , 2014, 20, 3730-3741.	3.3	31
599	Syntheses, structures, properties and DFT study of hybrid inorganic-organic architectures constructed from trinuclear lanthanide frameworks and Keggin-type polyoxometalates. <i>Dalton Transactions</i> , 2014, 43, 1906-1916.	3.3	73
600	Crystal engineering with coordination compounds of 2,6-dicarboxy-4-hydroxypyridine and 9-aminoacridine fragments driven by different nature of the face-to-face π - π stacking. <i>CrystEngComm</i> , 2014, 16, 1359-1377.	2.6	56
601	Relevant and unprecedented C-H...X cores. <i>Dalton Transactions</i> , 2014, 43, 6195-6211.	3.3	9
602	A dodecanuclear copper(^{II}) cage self-assembled from six dicopper building units. <i>Dalton Transactions</i> , 2014, 43, 4076-4085.	3.3	13
603	On the importance of non covalent interactions in the structure of coordination Cu(^{II}) and Co(^{II}) complexes of pyrazine- and pyridine-dicarboxylic acid derivatives: experimental and theoretical views. <i>CrystEngComm</i> , 2014, 16, 6149-6158.	2.6	57
604	Influence of ring size on the strength of carbon bonding complexes between anions and perfluorocycloalkanes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19192-19197.	2.8	41
605	A combined experimental and computational study of supramolecular assemblies in ternary copper(^{II}) complexes with a tetradentate N ₄ donor Schiff base and halides. <i>RSC Advances</i> , 2014, 4, 58643-58651.	3.6	29
606	An unusual nitroso-nitroso interaction in the coordination polymer structures of Ni(^{II}) and Co(^{II}) complexes with the 1,9-bis(benzotriazoloxyl)alkane system. <i>CrystEngComm</i> , 2014, 16, 654-666.	2.6	7
607	Crystal engineering with coordination compounds of NiII, CoII, and CrIII bearing dipicolinic acid driven by the nature of the noncovalent interactions. <i>CrystEngComm</i> , 2014, 16, 5352.	2.6	73
608	pH Dependent Formation of Unprecedented Water-Bromide Cluster in the Bromide Salts of PTP Assisted by Anion- π Interactions: Synthesis, Structure, and DFT Study. <i>Crystal Growth and Design</i> , 2014, 14, 747-755.	3.0	62
609	Thermodynamic Characterization of Halide- π Interactions in Solution Using α -Two-Wall-Aryl Extended Calix[4]pyrroles as Model System. <i>Journal of the American Chemical Society</i> , 2014, 136, 3208-3218.	13.7	96
610	Relation between the Catalytic Efficiency of the Synthetic Analogues of Catechol Oxidase with Their Electrochemical Property in the Free State and Substrate-Bound State. <i>Inorganic Chemistry</i> , 2014, 53, 8257-8269.	4.0	73
611	Experimental and Computational Study of Counterintuitive ClO ₄ ⁻ ...ClO ₄ ⁻ Interactions and the Interplay between π - π and Anion- π Interactions. <i>Crystal Growth and Design</i> , 2014, 14, 5812-5821.	3.0	113
612	Experimental and Theoretical Study of Aromaticity Effects in the Solid State Architecture on Squaric Acid Derivatives. <i>Crystal Growth and Design</i> , 2014, 14, 2578-2587.	3.0	24

#	ARTICLE	IF	CITATIONS
613	Role of ligand backbone of tridentate Schiff-base on complex nuclearity and bio-relevant catalytic activities of zinc(II) complexes: Experimental and theoretical investigations. <i>Inorganica Chimica Acta</i> , 2014, 421, 364-373.	2.4	28
614	Long-Range Effects in Anion-π Interactions: Their Crucial Role in the Inhibition Mechanism of <i>Mycobacterium Tuberculosis</i> Malate Synthase. <i>Chemistry - A European Journal</i> , 2014, 20, 6985-6990.	3.3	35
615	Small Cycloalkane (CN) ₂ C≡C(CN) ₂ Structures Are Highly Directional Non-covalent Carbon-Bond Donors. <i>Chemistry - A European Journal</i> , 2014, 20, 10245-10248.	3.3	89
616	Synthesis, X-ray characterization and DFT studies of bis-N-imidazolylpyrimidine salts: the prominent role of hydrogen bonding and anion-π interactions. <i>CrystEngComm</i> , 2014, 16, 9043-9053.	2.6	18
617	The influence of H-bonding on the π-ambidentate™ coordination behaviour of the thiocyanate ion to Cd(<i>scpi</i>): a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2014, 43, 8007-8015.	3.3	60
618	A combined experimental and theoretical study of the supramolecular self-assembly of Cu(II) malonate complex assisted by various weak forces and water dimer. <i>Journal of Solid State Chemistry</i> , 2014, 220, 149-156.	2.9	22
619	A Combined Theoretical and Cambridge Structural Database Study of π-Hole Pnictogen Bonding Complexes between Electron Rich Molecules and Both Nitro Compounds and Inorganic Bromides (YO ₂ Br, Y = N, P, and As). <i>Journal of Physical Chemistry A</i> , 2014, 118, 2827-2834.	2.5	92
620	Non-covalent sp ³ carbon bonding with ArCF ₃ is analogous to CH-π interactions. <i>Chemical Communications</i> , 2014, 50, 12626-12629.	4.1	86
621	Synthesis, Structure, and Binding Properties of Lipophilic Cavitands Based on a Calix[4]pyrrole-Resorcinarene Hybrid Scaffold. <i>Journal of Organic Chemistry</i> , 2014, 79, 5545-5557.	3.2	29
622	Combined Experimental and Theoretical Investigation of Ligand and Anion Controlled Complex Formation with Unprecedented Structural Features and Photoluminescence Properties of Zinc(II) Complexes. <i>Crystal Growth and Design</i> , 2014, 14, 4111-4123.	3.0	29
623	A new oxo centered basic p-chlorobenzoate bridging heterotrinnuclear complex, [Cr ₂ MnO(C ₇ H ₄ O ₂ Cl) ₆ (Py) ₃]C ₇ H ₅ O ₂ Cl: Synthesis, X-ray crystal structure and theoretical DFT study. <i>Polyhedron</i> , 2014, 81, 349-355.	2.2	6
624	Structural basis for molecular recognition, theoretical studies and anti-bacterial properties of three bis-uracil derivatives. <i>Tetrahedron</i> , 2014, 70, 6931-6937.	1.9	10
625	Computational study of anion recognition based on tetrel and hydrogen bonding interaction by calix[4]pyrrole derivatives. <i>Computational and Theoretical Chemistry</i> , 2014, 1038, 67-70.	2.5	67
626	On the Importance of Anion-π Interactions in the Mechanism of Sulfide:Quinone Oxidoreductase. <i>Chemistry - an Asian Journal</i> , 2013, 8, 2708-2713.	3.3	31
627	Structural characterization, recognition patterns and theoretical calculations of long-chain N-alkyl substituted purine and pyrimidine bases as ligands: On the importance of anion-π interactions. <i>Coordination Chemistry Reviews</i> , 2013, 257, 2705-2715.	18.8	42
628	Self-assembly cavitand precisely recognizing hexafluorosilicate: a concerted action of two coordination and twelve CH-F bonds. <i>Chemical Communications</i> , 2013, 49, 9018.	4.1	13
629	Experimental and theoretical study of N1-hexylcytosine and N1-hexylcytosinium nitrate: the crucial role of hydrophobic and anion-π interactions. <i>Tetrahedron Letters</i> , 2013, 54, 5355-5360.	1.4	8
630	Anion-π interactions in [S ₄ N ₃] ⁺ rings. <i>New Journal of Chemistry</i> , 2013, 37, 2636.	2.8	17

#	ARTICLE	IF	CITATIONS
631	On the Reliability of Pure and Hybrid DFT Methods for the Evaluation of Halogen, Chalcogen, and Pnicogen Bonds Involving Anionic and Neutral Electron Donors. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5201-5210.	5.3	243
632	Quadrupole moment versus Molecular Electrostatic Potential: Strange behavior of ethynyl-substituted benzenes. <i>Chemical Physics Letters</i> , 2013, 567, 60-65.	2.6	5
633	Tetrel-Bonding Interaction: Rediscovered Supramolecular Force?. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 12317-12321.	13.8	575
634	A Combined Experimental and Theoretical Investigation on the Role of Halide Ligands on the Catecholase-like Activity of Mononuclear Nickel(II) Complexes with a Phenol-Based Tridentate Ligand. <i>Inorganic Chemistry</i> , 2013, 52, 13442-13452.	4.0	83
635	Synthesis, crystal structure, magnetic property and DFT calculations of an unusual dinuclear μ_2 -alkoxido bridged iron(III) complex. <i>Dalton Transactions</i> , 2013, 42, 12274.	3.3	25
636	M ^{II} -Malonate Complexes (M = Mg, Cu, Ni and Co) Characterized by Layered Structures: Experimental Observation, Hirshfeld Surface Analysis and Theoretical Study. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 4679-4685.	2.0	54
637	Reversible switching of the electronic ground state in a pentacoordinated Cu(II) complex. <i>Chemical Communications</i> , 2013, 49, 7806.	4.1	13
638	Salt-bridge (sb) interactions at work: associative interactions of sb, π and anion- π in Cu(μ_2 -malonate)-2-aminopyridine-hexafluoridophosphate ternary system. <i>CrystEngComm</i> , 2013, 15, 686-696.	2.6	55
639	Influence of accompanying anions on supramolecular assembly and coordination geometry in HgII complexes with 8-aminoquinoline: experimental and theoretical studies. <i>CrystEngComm</i> , 2013, 15, 1404.	2.6	25
640	Halogen bonding versus chalcogen and pnicogen bonding: a combined Cambridge structural database and theoretical study. <i>CrystEngComm</i> , 2013, 15, 3137-3144.	2.6	206
641	Anion- π Interactions Involving [MX _n] ^{m+} Anions: A Comprehensive Theoretical Study. <i>ChemPhysChem</i> , 2013, 14, 145-154.	2.1	11
642	Polymorphism in hetero-metallic tri-nuclear CuII2CdII complexes of salicylaldimine ligand: Structural analysis and theoretical study. <i>Polyhedron</i> , 2013, 52, 1416-1424.	2.2	26
643	Encapsulation of anions: Macrocyclic receptors based on metal coordination and anion- π interactions. <i>Coordination Chemistry Reviews</i> , 2013, 257, 1716-1727.	18.8	113
644	Analysis of the contribution of the π -acidity of the s-tetrazine ring in the crystal packing of coordination polymers. <i>CrystEngComm</i> , 2013, 15, 3031.	2.6	33
645	Dinuclear and heptanuclear nickel(II) complexes: Anion coordination induced ligand arm hydrolysis and aggregation around a nickel(II) core. <i>Polyhedron</i> , 2013, 53, 32-39.	2.2	18
646	Is the Use of Diffuse Functions Essential for the Properly Description of Noncovalent Interactions Involving Anions?. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2651-2655.	2.5	38
647	Metallomacrocycles as anion receptors: combining hydrogen bonding and ion pair based hosts formed from Ag(I) salts and flexible bis- and tris-pyrimidine ligands. <i>Chemical Communications</i> , 2013, 49, 4944.	4.1	16
648	Different Nature of the Interactions between Anions and HAT(CN) ₆ : From Reversible Anion- π Complexes to Irreversible Electron-Transfer Processes (HAT(CN) ₆ =)		

#	ARTICLE	IF	CITATIONS
649	Use of Metalloligands [CuL] ($H_{2L} = \text{Salen Type Di-Schiff Bases}$) in the Formation of Heterobimetallic Copper(II)-Uranyl Complexes: Photophysical Investigations, Structural Variations, and Theoretical Calculations. <i>Inorganic Chemistry</i> , 2013, 52, 7508-7523.	4.0	79
650	On the Importance of Unprecedented Lone Pair \cdots Salt Bridge Interactions in Cu(II) \cdots Malonate \cdots 2-Amino-5-Chloropyridine \cdots Perchlorate Ternary System. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5802-5811.	2.5	34
651	A new benzimidazolium incorporated chemodosimeter affording dual chromogenic and fluorescence switch-on signaling for the selective targeting of cyanide. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2013, 76, 293-300.	1.6	2
652	Experimental and theoretical studies on the coordination chemistry of the N1-hexyl substituted pyrimidines (uracil, 5-fluorouracil and cytosine). <i>Dalton Transactions</i> , 2013, 42, 7631.	3.3	12
653	Differences in Nuclearity, Molecular Shapes, and Coordination Modes of Azide in the Complexes of Cd(II) and Hg(II) with a α -Metalloligand \cdots [CuL] ($H_{2L} = \text{Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 582 Td (<i>N</i>}$). <i>Theoretical Calculations. Inorganic Chemistry</i> , 2012, 51, 12407-12418.	4.0	51
654	Pnicogen \cdots complexes: theoretical study and biological implications. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14061.	2.8	113
655	Cis \cdots trans isomerism in diphenoxido bridged dicopper complexes: role of crystallized water to stabilize the cis isomer, variation in magnetic properties and conversion of both into a trinuclear species. <i>Dalton Transactions</i> , 2012, 41, 12200.	3.3	27
656	Understanding the Forces That Govern Packing: A Density Functional Theory and Structural Investigation of Anion \cdots Anion and Nonclassical C \cdots H \cdots Anion Interactions. <i>Inorganic Chemistry</i> , 2012, 51, 10334-10340.	4.0	32
657	Host \cdots Guest Supramolecular Interactions in the Coordination Compounds of 4,4'-Azobis(pyridine) with MnX_{2L} ($X = \text{NCS}^{\sup>}, \text{NCNCN}^{\sup>}, \text{and PF}_6^{\sup>}$): Structural Analyses and Theoretical Study. <i>Inorganic Chemistry</i> , 2012, 51, 1837-1851.	4.0	34
658	Experimental and theoretical study of thymine and cytosine derivatives: the crucial role of weak noncovalent interactions. <i>CrystEngComm</i> , 2012, 14, 5777.	2.6	17
659	Theoretical ab initio study of lone pair and anion \cdots interactions in fluorinated tropolones. <i>Computational and Theoretical Chemistry</i> , 2012, 998, 20-25.	2.5	7
660	Interplay between ion \cdots and Ar \cdots Van der Waals interactions. <i>Computational and Theoretical Chemistry</i> , 2012, 998, 51-56.	2.5	12
661	Feasibility of Single-Walled Carbon Nanotubes as Materials for CO_2 Adsorption: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 21083-21092.	3.1	32
662	Synthesis, X-ray characterization and computational studies of Cu(ii) complexes of N-pyrazolyl pyrimidine. <i>Dalton Transactions</i> , 2012, 41, 11161.	3.3	8
663	Complexes of Zinc(II) with N -imidazolyl \cdots and N -pyrazolylpyrimidine Donor Ligands: Synthesis, Crystal Structures, and Theoretical Study. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 3995-4003.	2.0	11
664	Effect of a methyl group on the spontaneous resolution of a square-pyramidal coordination compound: crystal packing and conglomerate formation. <i>CrystEngComm</i> , 2012, 14, 5854.	2.6	13
665	Anion Induced Formation of Supramolecular Associations Involving Lone pair \cdots and Anion \cdots Interactions in Co(II) Malonate Complexes: Experimental Observations, Hirshfeld Surface Analyses and DFT Studies. <i>Inorganic Chemistry</i> , 2012, 51, 3557-3571.	4.0	202
666	Tuning of the anion \cdots interaction. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	20

#	ARTICLE	IF	CITATIONS
667	Theoretical ab initio study of anion-π interactions in inorganic rings. <i>Chemical Physics Letters</i> , 2012, 530, 145-150.	2.6	17
668	Estimating ring strain energies in small carbocycles by means of the Bader's theory of atoms-in-molecules. <i>Chemical Physics Letters</i> , 2012, 536, 165-169.	2.6	27
669	Synthesis, X-ray characterization and computational Studies of N-imidazolyl and N-pyrazolyl pyrimidine derivatives. <i>Tetrahedron</i> , 2012, 68, 2374-2382.	1.9	8
670	RNAs' uracil quartet model with a non-essential metal ion. <i>Chemical Communications</i> , 2011, 47, 4646.	4.1	16
671	Design of a dual sensing highly selective cyanide chemodosimeter based on pyridinium ring chemistry. <i>New Journal of Chemistry</i> , 2011, 35, 57-60.	2.8	34
672	Unexpected Nonadditivity Effects in Anion-π Complexes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7849-7857.	2.5	23
673	RI-MP2 and MPWB1K Study of Anion-π Complexes: MPWB1K Performance and Some Additivity Aspects. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3012-3018.	5.3	26
674	Kinetics and mechanism of the oxidation of hydroxylamine by a {Mn ₃ O ₄ } ⁴⁺ core in aqueous acidic media. <i>Dalton Transactions</i> , 2011, 40, 9571.	3.3	2
675	Supramolecular Self-Assembly of M-IDA Complexes Involving Lone-Pair-π Interactions: Crystal Structures, Hirshfeld Surface Analysis, and DFT Calculations [H ₂ IDA = iminodiacetic acid, M = Cu(II), Ni(II)]. <i>Crystal Growth and Design</i> , 2011, 11, 3250-3265.	3.0	304
676	Substituent effects in halogen bonding complexes between aromatic donors and acceptors: a comprehensive ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20371.	2.8	92
677	On the directionality of anion-π interactions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5696.	2.8	78
678	Supramolecular assemblies involving anion-π and lone pair-π interactions: experimental observation and theoretical analysis. <i>CrystEngComm</i> , 2011, 13, 4519.	2.6	86
679	Radical cation (C ^{•+}) and radical anion (A ^{•-}) interactions with aromatic rings: energetic, orbitalic and spin density considerations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16698.	2.8	13
680	Self-assembly hexanuclear metallacontainer hosting halogenated guest species and sustaining structure of 3D coordination framework. <i>Chemical Communications</i> , 2011, 47, 1764-1766.	4.1	18
681	Theoretical ab initio study of substituted benzene trimer: Interplay between hydrogen bonding and π-π interactions. <i>Computational and Theoretical Chemistry</i> , 2011, 975, 106-110.	2.5	7
682	A Highly Selective Fluorescence Turn-on Probe for Zn ²⁺ Based on New Diaryloxadiazole Chelate. <i>Chemistry Letters</i> , 2011, 40, 1163-1164.	1.3	2
683	Anion-π Interactions in Flavoproteins. <i>Chemistry - an Asian Journal</i> , 2011, 6, 2316-2318.	3.3	52
684	Can lone pair-π and cation-π interactions coexist? A theoretical study. <i>Open Chemistry</i> , 2011, 9, 25-34.	1.9	14

#	ARTICLE	IF	CITATIONS
685	Cation-π and anion-π interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 440-459.	14.6	156
686	A methodological analysis for the assessment of non-covalent π interactions. Chemical Physics Letters, 2011, 508, 144-148.	2.6	23
687	Trinuclear and tetranuclear adduct formation between sodium perchlorate and copper(II) complexes of salicylaldehyde type ligands: Structural characterization and theoretical investigation. Inorganica Chimica Acta, 2011, 366, 219-226.	2.4	51
688	Synthesis and Crystal Structures of μ ₂ -Oxo- and μ ₂ -Hydroxo-Bridged Dinuclear Iron(III) Complexes with an N ₂ O Donor Ligand – A Theoretical Study on the Influence of Weak Forces on the Fe-O-Fe Bridging Angle. European Journal of Inorganic Chemistry, 2011, 2011, 2558-2566.	2.0	24
689	The Role of the Ethynyl Substituent on the π-π Stacking Affinity of Benzene: A Theoretical Study. ChemPhysChem, 2011, 12, 283-288.	2.1	3
690	Theoretical Study on Cooperativity Effects between Anion-π and Halogen-Bonding Interactions. ChemPhysChem, 2011, 12, 2742-2750.	2.1	79
691	Relevant Anion-π Interactions in Biological Systems: The Case of Urate Oxidase. Angewandte Chemie - International Edition, 2011, 50, 415-418.	13.8	164
692	Putting Anion-π Interactions Into Perspective. Angewandte Chemie - International Edition, 2011, 50, 9564-9583.	13.8	591
693	Anion...π, lone pair...π, and F...F interactions in nucleobase derivatives. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C600-C601.	0.3	0
694	Cooperativity in multiple unusual weak bonds. Theoretical Chemistry Accounts, 2010, 126, 1-14.	1.4	254
695	Cooperativity effects between non-covalent interactions: Are they important for Z-DNA stability?. Chemical Physics Letters, 2010, 485, 221-225.	2.6	13
696	New Chlorido(dimethyl sulfoxide)iridium(III) Complexes with N6-Substituted Adenines - Kinetic N(7) versus Thermodynamic N(9) Coordinated Adenine Isomers. European Journal of Inorganic Chemistry, 2010, 2010, 5617-5628.	2.0	10
697	A Combined Experimental and Theoretical Study of Anion-π Interactions in N ⁶ and N ⁹ -Decyladenine Salts. European Journal of Organic Chemistry, 2010, 2010, 5171-5180.	2.4	19
698	Hydrogen-bond assisted stabilization of the less favored conformation of a tridentate Schiff base ligand in dinuclear nickel(II) complex: An experimental and theoretical study. Inorganica Chimica Acta, 2010, 363, 3904-3913.	2.4	23
699	A novel fluoride selective optical chemosensor based on internal charge transfer signaling. Tetrahedron Letters, 2010, 51, 596-599.	1.4	33
700	Erroneous behaviour of the widely used MP2(full)/aug-cc-pVXZ (X=D,T) level of theory for evaluating the BSSE in ion-π complexes. Chemical Physics Letters, 2010, 489, 254-258.	2.6	20
701	Experimental and theoretical study of uracil derivatives: the crucial role of weak fluorine-π-fluorine noncovalent interactions. CrystEngComm, 2010, 12, 3758.	2.6	60
702	New 1,8-naphthyridine-based probes for the selective fluorescence signalling of toxic cadmium: synthesis, photophysical studies and molecular modelling. Supramolecular Chemistry, 2010, 22, 524-531.	1.2	4

#	ARTICLE	IF	CITATIONS
703	Self-Assembled Molecular Complexes and Coordination Polymers of Cd ^{II} , Hexamine, and Monocarboxylates: Structural Analysis and Theoretical Studies of Supramolecular Interactions. <i>Crystal Growth and Design</i> , 2010, 10, 1677-1687.	3.0	44
704	Substituent Effects in Ion ^π Interactions: Fine-Tuning via the Ethynyl Group. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1926-1930.	2.5	22
705	Supramolecular Assembly of Mg(II) Complexes Directed by Associative Lone Pair ^π /Anion ^π Lone Pair Interactions. <i>Journal of Physical Chemistry B</i> , 2010, 114, 4998-5009.	2.6	78
706	Lone pair ^π vs ^π interactions in 5-fluoro-1-hexyluracil and 1-hexyluracil: a combined crystallographic and computational study. <i>CrystEngComm</i> , 2010, 12, 362-365.	2.6	39
707	Very Long-Range Effects: Cooperativity between Anion ^π and Hydrogen-Bonding Interactions. <i>ChemPhysChem</i> , 2009, 10, 2256-2264.	2.1	80
708	Anion ^π , Lone Pair ^π , ^π and Hydrogen-Bonding Interactions in a Cu ^{II} Complex of 2 ⁺ Picolinate and Protonated 4,4'-Bipyridine: Crystal Structure and Theoretical Studies. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 2238-2246.	2.0	98
709	Interplay between anion ^π and hydrogen bonding interactions. <i>Journal of Computational Chemistry</i> , 2009, 30, 75-82.	3.3	79
710	Theoretical ab initio study of the interplay between hydrogen bonding, cation ^π and ^π interactions. <i>Theoretical Chemistry Accounts</i> , 2009, 122, 325-332.	1.4	31
711	Theoretical and crystallographic study of edge-to-face aromatic interactions between pyridine moieties and benzene. <i>Chemical Physics Letters</i> , 2009, 468, 280-285.	2.6	21
712	Interplay between cation ^π and hydrogen bonding interactions: Are non-additivity effects additive?. <i>Chemical Physics Letters</i> , 2009, 479, 316-320.	2.6	42
713	2-Aminopyrimidine Derivatives Exhibiting Anion ^π Interactions: A Combined Crystallographic and Theoretical Study. <i>Crystal Growth and Design</i> , 2009, 9, 2363-2376.	3.0	39
714	Simultaneous Interaction of Tetrafluoroethene with Anions and Hydrogen-Bond Donors: A Cooperativity Study. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1186-1194.	5.3	52
715	Counterintuitive Substituent Effect of the Ethynyl Group in Ion ^π Interactions. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10367-10375.	2.5	43
716	Energetic vs Synergetic Stability: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3266-3273.	2.5	52
717	1,2,4,5-Tetrazine: an unprecedented 1/4 ⁺ -coordination that enhances ability for anion ^π interactions. <i>Dalton Transactions</i> , 2009, , 2856.	3.3	126
718	Anion ^π Interactions in Four-Membered Rings. <i>Organic Letters</i> , 2009, 11, 1987-1990.	4.6	38
719	MP2 Study of synergistic effects between X ^π /H ^π (X = C,N,O) and ^π interactions. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 385-393.	1.4	62
720	High-Level Ab Initio Study of Anion ^π Interactions in Pyridine and Pyrazine Rings Coordinated to Ag ^I . <i>ChemPhysChem</i> , 2008, 9, 397-399.	2.1	53

#	ARTICLE	IF	CITATIONS
721	Crystallographic and Theoretical Evidence of Anion-π and Hydrogen-Bonding Interactions in a Squaramide-Nitrate Salt. <i>European Journal of Organic Chemistry</i> , 2008, 2008, 1864-1868.	2.4	49
722	On the importance of the inclusion of the basis set superposition error counterpoise correction during optimization of ion-π complexes. <i>Chemical Physics Letters</i> , 2008, 455, 325-330.	2.6	13
723	Interplay between cation-π and hydrogen bonding interactions. <i>Chemical Physics Letters</i> , 2008, 456, 257-261.	2.6	82
724	Interaction of positively and negatively charged aromatic hydrocarbons with benzene and triphenylene: Towards a model of pure organic insulators. <i>Chemical Physics Letters</i> , 2008, 460, 406-410.	2.6	36
725	Interplay between Edge-to-Face Aromatic and Hydrogen-Bonding Interactions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6017-6022.	2.5	24
726	MP2 Study of the Dual π/π Anion-Binding Affinity of Fluorinated Phthalic Acid Anhydrides. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1622-1626.	2.5	12
727	Theoretical and Crystallographic Study of the Dual π/π Anion Binding Affinity of Quinolizinium Cation. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1981-1989.	5.3	21
728	Coordination Complexes Exhibiting Anion-π Interactions: Synthesis, Structure, and Theoretical Studies. <i>Inorganic Chemistry</i> , 2008, 47, 5873-5881.	4.0	72
729	Anion-π Interactions in Bisadenine Derivatives: A Combined Crystallographic and Theoretical Study. <i>Inorganic Chemistry</i> , 2007, 46, 10724-10735.	4.0	104
730	Dual Cation and Anion Acceptor Molecules. The Case of the (1,6-C6H6)(1,6-C6F6)Cr(0) Complex. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3137-3142.	2.5	29
731	MP2 study of cooperative effects between cation-π, anion-π and π-π interactions. <i>New Journal of Chemistry</i> , 2007, 31, 556-560.	2.8	151
732	Induced-Polarization Energy Map: A Helpful Tool for Predicting Geometric Features of Anion-π Complexes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2098-2107.	5.3	20
733	A Combined Experimental and Theoretical Study of Anion-π Interactions in Bis(pyr-imidine) Salts. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 5821-5825.	2.4	29
734	A Theoretical Study of Anion-π Interactions in Seven-Membered Rings. <i>ChemPhysChem</i> , 2007, 8, 1182-1187.	2.1	47
735	MP2 study of anion-π complexes of trifluoro-s-triazine with tetrahedral and octahedral anions. <i>Chemical Physics Letters</i> , 2007, 438, 104-108.	2.6	29
736	Ab Initio Study of [n.n]Paracyclophane (n= 2, 3) Complexes with Cations: An Unprecedented Through-Space Substituent Effects. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5144-5148.	2.5	71
737	DABCO-Induced Self-Assembly of a Trisporphyrin Double-Decker Cage: Thermodynamic Characterization and Guest Recognition. <i>Journal of the American Chemical Society</i> , 2006, 128, 5560-5569.	13.7	96
738	MP2 Study of Cation-π Interactions (n= 1-4). <i>Journal of Physical Chemistry A</i> , 2006, 110, 9307-9309.	2.5	49

#	ARTICLE	IF	CITATIONS
739	Rational Design, Synthesis, and Application of a New Receptor for the Molecular Recognition of Tricarboxylate Salts in Aqueous Media. <i>Journal of Organic Chemistry</i> , 2006, 71, 7185-7195.	3.2	66
740	A theoretical ab initio study of [n.n]paracyclophane complexes with cations. <i>Chemical Physics Letters</i> , 2006, 417, 371-377.	2.6	12
741	Synthesis, X-ray structure analysis and computational studies of novel bis(thiocarbamoyl) disulfides with non-covalent Sâ€N and Sâ€S interactions. <i>Chemical Physics Letters</i> , 2006, 422, 234-239.	2.6	24
742	Affinity of ferrocene and (1,1â€²)(3,3â€²)[3,3]ferrocenophane to cations. <i>Chemical Physics Letters</i> , 2006, 424, 204-208.	2.6	4
743	Interplay Between Cation-â€€, Anion-â€€ and â€€-â€€ Interactions. <i>ChemPhysChem</i> , 2006, 7, 2487-2491.	2.1	145
744	Counterintuitive affinity of [2.2]paracyclophane to cations. <i>Chemical Physics Letters</i> , 2005, 408, 59-64.	2.6	14
745	Ab initio investigations of lithium insertion in boron and nitrogen-doped single-walled carbon nanotubes. <i>Chemical Physics Letters</i> , 2005, 411, 256-261.	2.6	24
746	A Theoretical ab initio Study of the Capacity of Several Binding Units for the Molecular Recognition of Anions. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 179-183.	2.4	74
747	DABCO-Directed Self-Assembly of Bisporphyrins (DABCO=1,4-Diazabicyclo[2.2.2]octane). <i>Chemistry - A European Journal</i> , 2005, 11, 2196-2206.	3.3	88
748	Anion-â€€ Interactions in Cyanuric Acids: A Combined Crystallographic and Computational Study. <i>Chemistry - A European Journal</i> , 2005, 11, 6560-6567.	3.3	167
749	Approximate Additivity of Anion-â€€ Interactions:â€‰ An Ab Initio Study on Anion-â€€, Anion-â€€ ₂ and Anion-â€€ ₃ Complexes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9341-9345.	2.5	101
750	Self-Assembly, Binding, and Dynamic Properties of Heterodimeric Porphyrin Macrocycles. <i>Journal of Organic Chemistry</i> , 2005, 70, 6616-6622.	3.2	39
751	Preparation, Solid-State Characterization, and Computational Study of a Crown Ether Attached to a Squaramide. <i>Organic Letters</i> , 2005, 7, 1437-1440.	4.6	35
752	Structure and Binding Energy of Anion-â€€ and Cation-â€€ Complexes:â€‰ A Comparison of MP2, RI-MP2, DFT, and DF-DFT Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4632-4637.	2.5	186
753	Electrophilic behaviour of 3-methyl-2-methylthio-1,3,4-thiadiazolium salts: A multimodal theoretical approach. <i>Arkivoc</i> , 2005, 2005, 415-437.	0.5	20
754	Self-assembly of [2]Rotaxane Exploiting Reversible Pt(II)- Pyridine Coordinate Bonds. <i>Molecules</i> , 2004, 9, 278-286.	3.8	8
755	Applicability of the ¹ H NMR chemical shifts computed by the ab initio/GIAO-HF methodology to the study of geometrical features of Zn-porphyrin dimers. <i>Tetrahedron Letters</i> , 2004, 45, 9387-9391.	1.4	8
756	Ab initio investigations of lithium diffusion in single-walled carbon nanotubes. <i>Chemical Physics</i> , 2004, 297, 85-91.	1.9	34

#	ARTICLE	IF	CITATIONS
757	Structural and energetic features of single-walled carbon nanotube junctions: a theoretical ab initio study. <i>Chemical Physics</i> , 2004, 303, 265-270.	1.9	19
758	Cation- π versus anion- π interactions: a comparative ab initio study based on energetic, electron charge density and aromatic features. <i>Chemical Physics Letters</i> , 2004, 392, 85-89.	2.6	74
759	Cation- π vs anion- π interactions: a complete π -orbital analysis. <i>Chemical Physics Letters</i> , 2004, 399, 220-225.	2.6	42
760	Conformational Preferences and Self-Template Macrocyclization of Squaramide-Based Foldable Modules. <i>Journal of Organic Chemistry</i> , 2004, 69, 2302-2308.	3.2	63
761	Cation- π versus Anion- π Interactions: Energetic, Charge Transfer, and Aromatic Aspects. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9423-9427.	2.5	171
762	Anion- π interactions in five-membered rings: a combined crystallographic and ab initio study. <i>Chemical Physics Letters</i> , 2003, 382, 534-540.	2.6	41
763	A Topological Analysis of the Electron Density in Anion- π Interactions. <i>ChemPhysChem</i> , 2003, 4, 1344-1348.	2.1	190
764	s-Tetrazine as a new binding unit in molecular recognition of anions. <i>Chemical Physics Letters</i> , 2003, 370, 7-13.	2.6	95
765	Intramolecular noncovalent force in cyclic amidines: nonbonded interaction between carbon atoms and heteroatoms. <i>Chemical Physics Letters</i> , 2003, 372, 489-496.	2.6	7
766	Lithium diffusion in single-walled carbon nanotubes: a theoretical study. <i>Chemical Physics Letters</i> , 2003, 374, 548-555.	2.6	55
767	Dual Binding Mode of s-Triazine to Anions and Cations. <i>Organic Letters</i> , 2003, 5, 2227-2229.	4.6	74
768	Weak C-H/ π Interaction Participates in the Diastereoselectivity of a Host-Guest Complex in the Presence of Six Strong Hydrogen Bonds. <i>Organic Letters</i> , 2003, 5, 1135-1138.	4.6	37
769	Anion- π interactions: must the aromatic ring be electron deficient?. <i>New Journal of Chemistry</i> , 2003, 27, 211-214.	2.8	116
770	Predicting Experimental Complexation-Induced Changes in ^1H NMR Chemical Shift for Complexes between Zinc-Porphyrins and Amines Using the ab Initio/GIAO-HF Methodology. <i>Organic Letters</i> , 2002, 4, 399-401.	4.6	30
771	Anion- π Interactions: Do They Exist?. <i>Angewandte Chemie</i> , 2002, 114, 3539-3542.	2.0	176
772	Quantification of Aromaticity in Oxocarbons: The Problem of the Fictitious "Nonaromatic" Reference System. <i>Chemistry - A European Journal</i> , 2002, 8, 433-438.	3.3	80
773	Anion- π Interactions: Do They Exist?. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 3389-3392.	13.8	690
774	Internal rotation in squaramide and related compounds. A theoretical ab initio study. <i>Theoretical Chemistry Accounts</i> , 2002, 108, 157-167.	1.4	2

#	ARTICLE	IF	CITATIONS
775	A theoretical study of aromaticity in squaramide complexes with anions. <i>Chemical Physics Letters</i> , 2002, 351, 115-120.	2.6	57
776	Counterintuitive interaction of anions with benzene derivatives. <i>Chemical Physics Letters</i> , 2002, 359, 486-492.	2.6	178
777	Predicting experimental complexation-induced changes in NMR chemical shift for complexes between metalloporphyrins and ligands using the Ab initio/GIAO-HF methodology. <i>Chemical Physics Letters</i> , 2002, 360, 72-78.	2.6	6
778	Quantification of Aromaticity in Oxocarbons: The Problem of the Fictitious "Nonaromatic" Reference System. <i>Chemistry - A European Journal</i> , 2002, 8, 433.	3.3	0
779	OPLS all-atom force field for squaramides and squaric acid. <i>Chemical Physics Letters</i> , 2001, 350, 331-338.	2.6	12
780	A topological analysis of charge density in complexes between derivatives of squaric acid and ammonium cation. <i>Chemical Physics Letters</i> , 2001, 339, 369-374.	2.6	9
781	The resonance model in amides: a combined crystallographic and ab initio investigation. <i>New Journal of Chemistry</i> , 2001, 25, 259-261.	2.8	15
782	Squaramide as a binding unit in molecular recognition. <i>Chemical Physics Letters</i> , 2000, 326, 247-254.	2.6	62
783	A theoretical study of aromaticity in squaramide and oxocarbons. <i>Tetrahedron Letters</i> , 2000, 41, 2001-2005.	1.4	74
784	Ab initio calculations on zinc porphyrins complexed to amines: geometrical details and NMR chemical shifts. <i>Computational and Theoretical Chemistry</i> , 2000, 531, 381-386.	1.5	14
785	Squaramido-based receptors: applicability of molecular interaction potential to molecular recognition of polyalkylammonium compounds. <i>Theoretical Chemistry Accounts</i> , 2000, 104, 50-66.	1.4	9
786	OPLS all-atom force field for carbohydrates. <i>Journal of Computational Chemistry</i> , 1997, 18, 1955-1970.	3.3	619
787	OPLS all-atom force field for carbohydrates. , 1997, 18, 1955.		2
788	OPLS all-atom force field for carbohydrates. <i>Journal of Computational Chemistry</i> , 1997, 18, 1955-1970.	3.3	26
789	On the Mechanism of Lithiation of Hydric Aromatics: Direct NMR Evidence for Short H ⁺ Li Contacts in Mixed Aggregates. <i>Journal of Organic Chemistry</i> , 1996, 61, 5194-5195.	3.2	37
790	Molecular Recognition of Carbohydrates: Interaction of Diols with Acetate Ion. , 1996, , 115-126.		2
791	Solid-State Redox Chemistry: Preparation of 1,4-Naphthoquinone, Hydroquinone, and the Corresponding Mixed Quinhydrone in the Solid State. <i>Journal of Chemical Education</i> , 1995, 72, 63.	2.3	14
792	Predicting Directed Lithiations by Means of MNDO-Determined Agostic Interaction Parameters and Proximity Features. Peri Lithiation of Polyhydric Phenolic Compounds. <i>Journal of the American Chemical Society</i> , 1995, 117, 1105-1116.	13.7	28

#	ARTICLE	IF	CITATIONS
793	Origin of the regioselective lithiation of 1,3-disubstituted heteroatom aromatics. MNDO evidence for bidentate complexation. <i>Journal of the American Chemical Society</i> , 1992, 114, 9093-9100.	13.7	46
794	Double group-transfer reactions: a theoretical (AM1) approach. <i>Journal of Organic Chemistry</i> , 1992, 57, 6731-6735.	3.2	12
795	The generation of C,O,O-trilithiated derivatives of dihydric phenols. <i>Tetrahedron Letters</i> , 1991, 32, 7313-7316.	1.4	8
796	Exploring 3D non-interpenetrated metal-organic framework with malonate-bridged Co(II) coordination polymer: structural elucidation and theoretical study. <i>Phase Transitions</i> , 0, , 1-12.	1.3	0
797	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 $\hat{\pm}$ -effect. <i>CrystEngComm</i> , 0, , .	2.6	2
798	Modified-amino acid/peptide pyrimidine analogs: synthesis, structural characterization and DFT studies of N-(pyrimidyl)gabapentine and N-(pyrimidyl)baclofen. <i>New Journal of Chemistry</i> , 0, , .	2.8	1
799	Anion- $\hat{\Gamma}$ Catalysis Enabled by the Mechanical Bond**. <i>Angewandte Chemie</i> , 0, , .	2.0	0
800	Combined crystallographic and computational investigation of the solvent disorder present in a new tipiracil hydrochloride methanol solvate-hydrate. <i>CrystEngComm</i> , 0, , .	2.6	1
801	Static discrete disorder in the crystal structure of iododiflunisal: on the importance of hydrogen bond, halogen bond and $\hat{\Gamma}$ -stacking interactions. <i>CrystEngComm</i> , 0, , .	2.6	3
802	Centroid-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. <i>CrystEngComm</i> , 0, , .	2.6	5