Antonio Frontera

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1360434/publications.pdf

Version: 2024-02-01

802	27,203	9264	17105
papers	citations	74 h-index	122 g-index

836	836	836	12736
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Anionâ€“Ï€ Interactions: Do They Exist?. Angewandte Chemie - International Edition, 2002, 41, 3389-3392.	13.8	690
2	OPLS all-atom force field for carbohydrates. Journal of Computational Chemistry, 1997, 18, 1955-1970.	3.3	619
3	Putting Anionâ€“Ï€ Interactions Into Perspective. Angewandte Chemie - International Edition, 2011, 50, 9564-9583.	13.8	591
4	Tetrelâ€Bonding Interaction: Rediscovered Supramolecular Force?. Angewandte Chemie - International Edition, 2013, 52, 12317-12321.	13.8	575
5	The Bright Future of Unconventional Ïƒ/Ï€â€Hole Interactions. ChemPhysChem, 2015, 16, 2496-2517.	2.1	569
6	Definition of the chalcogen bond (IUPAC Recommendations 2019). Pure and Applied Chemistry, 2019, 91, 1889-1892.	1.9	322
7	Supramolecular Self-Assembly of M-IDA Complexes Involving Lone-PairÂ·Â·Â·Ï€ Interactions: Crystal Structures, Hirshfeld Surface Analysis, and DFT Calculations [H₂IDA = iminodiacetic acid, M = Cu(II), Ni(II)]. Crystal Growth and Design, 2011, 11, 3250-3265.	3.0	304
8	Aerogen Bonding Interaction: A New Supramolecular Force?. Angewandte Chemie - International Edition, 2015, 54, 7340-7343.	13.8	294
9	Not Only Hydrogen Bonds: Other Noncovalent Interactions. Crystals, 2020, 10, 180.	2.2	289
10	Cooperativity in multiple unusual weak bonds. Theoretical Chemistry Accounts, 2010, 126, 1-14.	1.4	254
11	On the Reliability of Pure and Hybrid DFT Methods for the Evaluation of Halogen, Chalcogen, and Pnicogen Bonds Involving Anionic and Neutral Electron Donors. Journal of Chemical Theory and Computation, 2013, 9, 5201-5210.	5.3	243
12	Halogen bonding versuschalcogen and pnicogen bonding: a combined Cambridge structural database and theoretical study. CrystEngComm, 2013, 15, 3137-3144.	2.6	206
13	Anion Induced Formation of Supramolecular Associations Involving Lone pairâˆ’Ï€ and Anionâˆ’Ï€ Interactions in Co(II) Malonate Complexes: Experimental Observations, Hirshfeld Surface Analyses and DFT Studies. Inorganic Chemistry, 2012, 51, 3557-3571.	4.0	202
14	A Topological Analysis of the Electron Density in Anion-Ï€ Interactions. ChemPhysChem, 2003, 4, 1344-1348.	2.1	190
15	Tetrel Bonding Interactions. Chemical Record, 2016, 16, 473-487.	5.8	188
16	A thorough anionâ€“Ï€ interaction study in biomolecules: on the importance of cooperativity effects. Chemical Science, 2016, 7, 1038-1050.	7.4	188
17	Structure and Binding Energy of Anionâˆ’Ï€ and Cationâˆ’Ï€ Complexes:Â A Comparison of MP2, RI-MP2, DFT, and DF-DFT Methods. Journal of Physical Chemistry A, 2005, 109, 4632-4637.	2.5	186
18	Counterintuitive interaction of anions with benzene derivatives. Chemical Physics Letters, 2002, 359, 486-492.	2.6	178

#	Article	IF	Citations
19	Anionâ€“Ï€ Interactions: Do They Exist?. Angewandte Chemie, 2002, 114, 3539-3542.	2.0	176
20	Cationâˆ’Ï€ versus Anionâˆ’Ï€ Interactions:Â Energetic, Charge Transfer, and Aromatic Aspects. Journal of Physical Chemistry A, 2004, 108, 9423-9427.	2.5	171
21	Anion-Ï€ Interactions in Cyanuric Acids: A Combined Crystallographic and Computational Study. Chemistry - A European Journal, 2005, 11, 6560-6567.	3.3	167
22	Relevant Anionâ€“Ï€ Interactions in Biological Systems: The Case of Urate Oxidase. Angewandte Chemie - International Edition, 2011, 50, 415-418.	13.8	164
23	Recent developments in the crystal engineering of diverse coordination modes (0â€“12) for Keggin-type polyoxometalates in hybrid inorganicâ€“organic architectures. Coordination Chemistry Reviews, 2014, 275, 1-18.	18.8	159
24	Cationâ€“Ï€ and anionâ€“Ï€ interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 440-459.	14.6	156
25	MP2 study of cooperative effects between cationâ€“Ï€, anionâ€“Ï€ and Ï€â€“Ï€ interactions. New Journal of Chemistry, 2007, 31, 556-560.	2.8	151
26	Tetrel bonding interactions at work: Impact on tin and lead coordination compounds. Coordination Chemistry Reviews, 2019, 384, 107-125.	18.8	148
27	Interplay Between Cation-Ï€, Anion-Ï€ and Ï€-Ï€ Interactions. ChemPhysChem, 2006, 7, 2487-2491.	2.1	145
28	Tuning the topology of hybrid inorganicâ€“organic materials based on the study of flexible ligands and negative charge of polyoxometalates: A crystal engineering perspective. Coordination Chemistry Reviews, 2016, 309, 84-106.	18.8	140
29	Spodium Bonds: Noncovalent Interactions Involving Groupâ€…12 Elements. Angewandte Chemie - International Edition, 2020, 59, 17482-17487.	13.8	136
30	Directionality of Ï€-holes in nitro compounds. Chemical Communications, 2015, 51, 1491-1493.	4.1	130
31	1,2,4,5-Tetrazine: an unprecedented Î¼4-coordination that enhances ability for anionâ‹¯Ï€ interactions. Dalton Transactions, 2009, , 2856.	3.3	126
32	Unprecedented structural variations in trinuclear mixed valence Co(<scp>ii</scp>/<scp>iii</scp>) complexes: theoretical studies, pnicogen bonding interactions and catecholase-like activities. Dalton Transactions, 2015, 44, 3862-3876.	3.3	124
33	Anionâ€“Ï€ interactions: must the aromatic ring be electron deficient?. New Journal of Chemistry, 2003, 27, 211-214.	2.8	116
34	A survey of the different roles of polyoxometalates in their interaction with amino acids, peptides and proteins. Dalton Transactions, 2017, 46, 6812-6829.	3.3	116
35	Pnicogenâ€“Ï€ complexes: theoretical study and biological implications. Physical Chemistry Chemical Physics, 2012, 14, 14061.	2.8	113
36	Encapsulation of anions: Macrocyclic receptors based on metal coordination and anionâ€“Ï€ interactions. Coordination Chemistry Reviews, 2013, 257, 1716-1727.	18.8	113

#	Article	IF	Citations
37	Experimental and Computational Study of Counterintuitive ClO₄^{â€“}Â·Â·Â·ClO₄^{â€“} Interactions and the Interplay between Ï€⁺â€“Ï€ and AnionÂ·Â·Â·Ï€⁺ Interactions. Crystal Growth and Design, 2014, 14, 5812-5821.	3.0	113
38	A Ni-based MOF for selective detection and removal of Hg²⁺ in aqueous medium: a facile strategy. Dalton Transactions, 2017, 46, 1943-1950.	3.3	106
39	Anionâˆ’Ï€ Interactions in Bisadenine Derivatives:â€‰ A Combined Crystallographic and Theoretical Study. Inorganic Chemistry, 2007, 46, 10724-10735.	4.0	104
40	Approximate Additivity of Anionâˆ’Ï€ Interactions:â€‰ An Ab Initio Study on Anionâˆ’Ï€, Anionâˆ’Ï€2 and Anionâˆ’Ï€3 Complexes. Journal of Physical Chemistry A, 2005, 109, 9341-9345.	2.5	101
41	Different Nature of the Interactions between Anions and HAT(CN)₆: From Reversible Anionâˆ’Ï€ Complexes to Irreversible Electron-Transfer Processes (HAT(CN)₆ =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T		
42	Towards design strategies for anionâ€“Ï€ interactions in crystal engineering. CrystEngComm, 2016, 18, 10-23.	2.6	101
43	Anionâ€“Ï€, Loneâ€Pairâ€“Ï€, Ï€â€“Ï€ and Hydrogenâ€Bonding Interactions in a Cu^{II} Complex of 2â€Picolinate and Protonated 4,4â€²â€Bipyridine: Crystal Structure and Theoretical Studies. European Journal of Inorganic Chemistry, 2009, 2009, 2238-2246.	2.0	98
44	Ï€-Hole aerogen bonding interactions. Physical Chemistry Chemical Physics, 2015, 17, 24748-24753.	2.8	98
45	Rationalization of Noncovalent Interactions within Six New M^{II}/8-Aminoquinoline Supramolecular Complexes (M^{II} = Mn, Cu, and Cd): A Combined Experimental and Theoretical DFT Study. Crystal Growth and Design, 2015, 15, 1351-1361.	3.0	97
46	DABCO-Induced Self-Assembly of a Trisporphyrin Double-Decker Cage:Â Thermodynamic Characterization and Guest Recognition. Journal of the American Chemical Society, 2006, 128, 5560-5569.	13.7	96
47	Thermodynamic Characterization of Halideâˆ’Ï€ Interactions in Solution Using â€œTwo-Wallâ€•Aryl Extended Calix[4]pyrroles as Model System. Journal of the American Chemical Society, 2014, 136, 3208-3218.	13.7	96
48	s-Tetrazine as a new binding unit in molecular recognition of anions. Chemical Physics Letters, 2003, 370, 7-13.	2.6	95
49	Design of Lead(II) Metalâ€“Organic Frameworks Based on Covalent and Tetrel Bonding. Chemistry - A European Journal, 2015, 21, 17951-17958.	3.3	93
50	Application of a novel 2D cadmium(<scp>ii</scp>)-MOF in the formation of a photo-switch with a substantial onâ€“off ratio. Chemical Communications, 2015, 51, 12974-12976.	4.1	93
51	Substituent effects in halogen bonding complexes between aromatic donors and acceptors: a comprehensive ab initio study. Physical Chemistry Chemical Physics, 2011, 13, 20371.	2.8	92
52	A Combined Theoretical and Cambridge Structural Database Study of Ï€-Hole Pnicogen Bonding Complexes between Electron Rich Molecules and Both Nitro Compounds and Inorganic Bromides (YO₂Br, Y = N, P, and As). Journal of Physical Chemistry A, 2014, 118, 2827-2834.	2.5	92
53	Small Cycloalkane (CN)₂Cï£¿C(CN)₂ Structures Are Highly Directional Nonâ€covalent Carbonâ€Bond Donors. Chemistry - A European Journal, 2014, 20, 10245-10248.	3.3	89
54	DABCO-Directed Self-Assembly of Bisporphyrins (DABCO=1,4-Diazabicyclo[2.2.2]octane). Chemistry - A European Journal, 2005, 11, 2196-2206.	3.3	88

#	Article	IF	Citations
55	Supramolecular assemblies involving anionâ€“Ï€ and lone pairâ€“Ï€ interactions: experimental observation and theoretical analysis. CrystEngComm, 2011, 13, 4519.	2.6	86
56	Non-covalent sp³carbon bonding with ArCF₃is analogous to CHâ€“Ï€ interactions. Chemical Communications, 2014, 50, 12626-12629.	4.1	86
57	Hydrogen Bond, Ï€â€“Ï€, and CHâ€“Ï€ Interactions Governing the Supramolecular Assembly of Some Hydrazone Ligands and Their Mn^{II} Complexes â€“ Structural and Theoretical Interpretation. European Journal of Inorganic Chemistry, 2015, 2015, 1958-1972.	2.0	84
58	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. Inorganic Chemistry, 2013, 52, 13442-13452.	4.0	83
59	Ïƒ/Ï€-Hole noble gas bonding interactions: Insights from theory and experiment. Coordination Chemistry Reviews, 2020, 404, 213112.	18.8	83
60	Interplay between cation-Ï€ and hydrogen bonding interactions. Chemical Physics Letters, 2008, 456, 257-261.	2.6	82
61	3-Picoline Mediated Self-Assembly of M(II)â€“Malonate Complexes (M = Ni/Co/Mn/Mg/Zn/Cu) Assisted by Various Weak Forces Involving Lone Pairâˆ˜Ï€, Ï€â€“Ï€, and AnionÂ·Â·Â·Ï€â€“Hole Interactions. Journal of Physical Chemistry B, 2014, 118, 14713-14726.	2.6	81
62	Regiumâ€“Ï€ bonds: An Unexplored Link between Noble Metal Nanoparticles and Aromatic Surfaces. Chemistry - A European Journal, 2018, 24, 7228-7234.	3.3	81
63	Quantification of Aromaticity in Oxocarbons: The Problem of the Fictitious â€œNonaromaticâ€•Reference System. Chemistry - A European Journal, 2002, 8, 433-438.	3.3	80
64	Very Longâ€Range Effects: Cooperativity between Anionâ€“Ï€ and Hydrogenâ€Bonding Interactions. ChemPhysChem, 2009, 10, 2256-2264.	2.1	80
65	Interplay between anionâ€Ï€ and hydrogen bonding interactions. Journal of Computational Chemistry, 2009, 30, 75-82.	3.3	79
66	Theoretical Study on Cooperativity Effects between Anionâ€“Ï€ and Halogenâ€Bonding Interactions. ChemPhysChem, 2011, 12, 2742-2750.	2.1	79
67	Use of Metalloligands [CuL] (H₂L = Salen Type Di-Schiff Bases) in the Formation of Heterobimetallic Copper(II)-Uranyl Complexes: Photophysical Investigations, Structural Variations, and Theoretical Calculations. Inorganic Chemistry, 2013, 52, 7508-7523.	4.0	79
68	Supramolecular Assembly of Mg(II) Complexes Directed by Associative Lone Pairâˆ˜Ï€/Ï€âˆ˜Ï€/Ï€âˆ˜Anionâˆ˜Ï€/Ï€âˆ˜Lone Pair Interactions. Journal of Physical Chemistry B, 2010, 114, 4998-5009.	2.6	78
69	On the directionality of anionâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2011, 13, 5696.	2.8	78
70	Exploration of CHâ‹¯Ï€ interactions involving the Ï€-system of pseudohalide coligands in metal complexes of a Schiff-base ligand. CrystEngComm, 2015, 17, 4680-4690.	2.6	78
71	On the importance of tetrel bonding interactions in lead(<scp>ii</scp>) complexes with (iso)nicotinohydrazide based ligands and several anions. Dalton Transactions, 2016, 45, 10708-10716.	3.3	78
72	Synergistic Anionâ€“(Ï€)_nâ€“Ï€ Catalysis on Ï€-Stacked Foldamers. Journal of the American Chemical Society, 2018, 140, 4884-4892.	13.7	78

#	Article	IF	Citations
73	On the preferences of five-membered chelate rings in coordination chemistry: insights from the Cambridge Structural Database and theoretical calculations. Dalton Transactions, 2019, 48, 5476-5490.	3.3	78
74	A Strategy to Synthesize Molecular Knots and Links Using the Hydrophobic Effect. Journal of the American Chemical Society, 2018, 140, 12442-12450.	13.7	75
75	A theoretical study of aromaticity in squaramide and oxocarbons. Tetrahedron Letters, 2000, 41, 2001-2005.	1.4	74
76	Dual Binding Mode ofs-Triazine to Anions and Cations. Organic Letters, 2003, 5, 2227-2229.	4.6	74
77	Cation-Ï€ versus anion-Ï€ interactions: a comparative ab initio study based on energetic, electron charge density and aromatic features. Chemical Physics Letters, 2004, 392, 85-89.	2.6	74
78	A Theoretical ab initio Study of the Capacity of Several Binding Units for the Molecular Recognition of Anions. European Journal of Organic Chemistry, 2005, 2005, 179-183.	2.4	74
79	Anionâ^Ï€ Catalysis on Fullerenes. Journal of the American Chemical Society, 2017, 139, 13296-13299.	13.7	74
80	Syntheses, structures, properties and DFT study of hybrid inorganicâ€“organic architectures constructed from trinuclear lanthanide frameworks and Keggin-type polyoxometalates. Dalton Transactions, 2014, 43, 1906-1916.	3.3	73
81	Crystal engineering with coordination compounds of NiII, CoII, and CrIII bearing dipicolinic acid driven by the nature of the noncovalent interactions. CrystEngComm, 2014, 16, 5352.	2.6	73
82	Relation between the Catalytic Efficiency of the Synthetic Analogues of Catechol Oxidase with Their Electrochemical Property in the Free State and Substrate-Bound State. Inorganic Chemistry, 2014, 53, 8257-8269.	4.0	73
83	Coordination Complexes Exhibiting AnionÂ·Â·Â·Ï€ Interactions: Synthesis, Structure, and Theoretical Studies. Inorganic Chemistry, 2008, 47, 5873-5881.	4.0	72
84	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. Inorganic Chemistry, 2016, 55, 8502-8513.	4.0	72
85	NO3â^' anions can act as Lewis acid in the solid state. Nature Communications, 2017, 8, 14522.	12.8	72
86	Quantifying conventional Câ€“Hâ‹¯Ï€(aryl) and unconventional Câ€“Hâ‹¯Ï€(chelate) interactions in dinuclear Cu(<scp>ii</scp>) complexes: experimental observations, Hirshfeld surface and theoretical DFT study. New Journal of Chemistry, 2018, 42, 10202-10213.	2.8	72
87	Ab Initio Study of [n.n]Paracyclophane (n= 2, 3) Complexes with Cations:Â Unprecedented Through-Space Substituent Effects. Journal of Physical Chemistry A, 2006, 110, 5144-5148.	2.5	71
88	Concurrent agostic and tetrel bonding interactions in lead(<scp>ii</scp>) complexes with an isonicotinohydrazide based ligand and several anions. Dalton Transactions, 2016, 45, 4965-4969.	3.3	71
89	Importance of Râ€“CF₃Â·Â·Â·O Tetrel Bonding Interactions in Biological Systems. Journal of Physical Chemistry A, 2017, 121, 5371-5376.	2.5	69
90	RCH3Â·Â·Â·O Interactions in Biological Systems: Are They Trifurcated H-Bonds or Noncovalent Carbon Bonds?. Crystals, 2016, 6, 26.	2.2	68

#	Article	IF	Citations
91	Ïƒâ€Hole Opposite to a Lone Pair: Unconventional Pnicogen Bonding Interactions between ZF₃ (Z=N, P, As, and Sb) Compounds and Several Donors. ChemPhysChem, 2016, 17, 1608-1614.	2.1	68
92	Screening polymorphism in a Ni(<scp>ii</scp>) metalâ€“organic framework: experimental observations, Hirshfeld surface analyses and DFT studies. CrystEngComm, 2018, 20, 746-754.	2.6	68
93	A Series of Lanthanide-Based Metalâ€“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. Inorganic Chemistry, 2019, 58, 7760-7774.	4.0	68
94	Computational study of anion recognition based on tetrel and hydrogen bonding interaction by calix[4]pyrrole derivatives. Computational and Theoretical Chemistry, 2014, 1038, 67-70.	2.5	67
95	Ï€-Hole Interactions Involving Nitro Compounds: Directionality of Nitrate Esters. Crystal Growth and Design, 2016, 16, 5520-5524.	3.0	67
96	Rational Design, Synthesis, and Application of a New Receptor for the Molecular Recognition of Tricarboxylate Salts in Aqueous Media. Journal of Organic Chemistry, 2006, 71, 7185-7195.	3.2	66
97	A Cd(<scp>ii</scp>)-based MOF as a photosensitive Schottky diode: experimental and theoretical studies. Dalton Transactions, 2017, 46, 11239-11249.	3.3	66
98	Conformational Preferences and Self-Template Macrocyclization of Squaramide-Based Foldable Modules. Journal of Organic Chemistry, 2004, 69, 2302-2308.	3.2	63
99	Theoretical Study on the Dual Behavior of XeO₃ and XeF₄ toward Aromatic Rings: Lone Pairâ€“Ï€ versus Aerogenâ€“Ï€ Interactions. ChemPhysChem, 2015, 16, 3625-3630.	2.1	63
100	Ï€â€“hole interactions at work: crystal engineering with nitro-derivatives. CrystEngComm, 2017, 19, 1933-1937.	2.6	63
101	Pbâ‹¯X (X = N, S, I) tetrel bonding interactions in Pb(<scp>ii</scp>) complexes: X-ray characterization, Hirshfeld surfaces and DFT calculations. CrystEngComm, 2018, 20, 2812-2821.	2.6	63
102	Squaramide as a binding unit in molecular recognition. Chemical Physics Letters, 2000, 326, 247-254.	2.6	62
103	MP2 Study of synergistic effects between Xâ€“H/Ï€ (X = C,N,O) and Ï€â€“Ï€ interactions. Theoretical Chemistry Accounts, 2008, 120, 385-393.	1.4	62
104	pH Dependent Formation of Unprecedented Waterâ€“Bromide Cluster in the Bromide Salts of PTP Assisted by Anionâ‹¯Ï€ Interactions: Synthesis, Structure, and DFT Study. Crystal Growth and Design, 2014, 14, 747-755.	3.0	62
105	DFT prediction of band gap in organic-inorganic metal halide perovskites: An exchange-correlation functional benchmark study. Chemical Physics, 2019, 516, 225-231.	1.9	62
106	Pnictogen-bonding catalysis: brevetoxin-type polyether cyclizations. Chemical Science, 2020, 11, 7086-7091.	7.4	62
107	Halogen and Chalcogen Bond Energies Evaluated Using Electron Density Properties. ChemPhysChem, 2020, 21, 26-31.	2.1	61
108	Heteronuclear cobalt(<scp>iii</scp>)/sodium complexes with salen type compartmental Schiff base ligands: methylene spacer regulated variation in nuclearity. Dalton Transactions, 2018, 47, 331-347.	3.3	61

#	Article	IF	Citations
109	Experimental and theoretical study of uracil derivatives: the crucial role of weak fluorineâ€“fluorine noncovalent interactions. CrystEngComm, 2010, 12, 3758.	2.6	60
110	The influence of H-bonding on the â€˜ambidentateâ€™ coordination behaviour of the thiocyanate ion to Cd(<scp>II</scp>): a combined experimental and theoretical study. Dalton Transactions, 2014, 43, 8007-8015.	3.3	60
111	Estimation of conventional Câ€“Hâ‹¯Ï€ (arene), unconventional Câ€“Hâ‹¯Ï€ (chelate) and Câ€“Hâ‹¯Ï€ (thiocyanate) interactions in hetero-nuclear nickel(<scp>II</scp>)â€“cadmium(<scp>II</scp>) complexes with a compartmental Schiff base. Dalton Transactions, 2017, 46, 5384-5397.	3.3	60
112	Anionâ‹…â‹…â‹…Anion Interactions Involving Ïƒâ€Holes of Perrhenate, Pertechnetate and Permanganate Anions. ChemPhysChem, 2021, 22, 2281-2285.	2.1	60
113	Molecular Electrostatic Potential and Noncovalent Interactions in Derivatives of Group 8 Elements. Angewandte Chemie - International Edition, 2021, 60, 20723-20727.	13.8	58
114	A theoretical study of aromaticity in squaramide complexes with anions. Chemical Physics Letters, 2002, 351, 115-120.	2.6	57
115	On the importance of non covalent interactions in the structure of coordination Cu(<scp>II</scp>) and Co(<scp>II</scp>) complexes of pyrazine- and pyridine-dicarboxylic acid derivatives: experimental and theoretical views. CrystEngComm, 2014, 16, 6149-6158.	2.6	57
116	Nature of Noncovalent Carbonâ€Bonding Interactions Derived from Experimental Chargeâ€Density Analysis. ChemPhysChem, 2015, 16, 2530-2533.	2.1	57
117	Crystal engineering with coordination compounds of 2,6-dicarboxy-4-hydroxypyridine and 9-aminoacridine fragments driven by different nature of the face-to-face Ï€â‹¯Ï€ stacking. CrystEngComm, 2014, 16, 1359-1377.	2.6	56
118	Three mononuclear octahedral cobalt(III) complexes with salicylaldimine Schiff bases: Synthesis, characterization, phenoxazinone synthase mimicking activity and DFT study on supramolecular interactions. Polyhedron, 2016, 112, 6-17.	2.2	56
119	A Schiff base platform: structures, sensing of Zn(<scp>II</scp>) and PPi in aqueous medium and anticancer activity. Dalton Transactions, 2017, 46, 9498-9510.	3.3	56
120	Lithium diffusion in single-walled carbon nanotubes: a theoretical study. Chemical Physics Letters, 2003, 374, 548-555.	2.6	55
121	Salt-bridgeâ€“Ï€ (sbâ€“Ï€) interactions at work: associative interactions of sbâ€“Ï€, Ï€â€“Ï€ and anionâ€“Ï€ in Cu(<scp>II</scp>)-malonateâ€“2-aminopyridineâ€“hexafluoridophosphate ternary system. CrystEngComm, 2013, 15, 686-696.	2.6	55
122	M^{II}â€“Malonate Complexes (M = Mg, Cu, Ni and Co) Characterized by Layered Structures: Experimental Observation, Hirshfeld Surface Analysis and Theoretical Study. European Journal of Inorganic Chemistry, 2013, 2013, 4679-4685.	2.0	54
123	A crystalline sponge based on dispersive forces suitable for X-ray structure determination of included molecular guests. Chemical Science, 2015, 6, 5466-5472.	7.4	54
124	Benzyl Dihydrazone versus Thiosemicarbazone Schiff Base: Effects on the Supramolecular Arrangement of Cobalt Thiocyanate Complexes and the Generation of CoN₆ and CoN₄S₂ Coordination Spheres. European Journal of Inorganic Chemistry, 2017, 2017, 4763-4772.	2.0	54
125	A series of 3D lanthanide coordination polymers decorated with a rigid 3,5-pyridinedicarboxylic acid linker: syntheses, structural diversity, DFT study, Hirshfeld surface analysis, luminescence and magnetic properties. Dalton Transactions, 2018, 47, 12318-12336.	3.3	54
126	Recurrent Ï€â€“Ï€ stacking motifs in three new 4,5-dihydropyrazolylâ€“thiazoleâ€“coumarin hybrids: X-ray characterization, Hirshfeld surface analysis and DFT calculations. New Journal of Chemistry, 2020, 44, 14592-14603.	2.8	54

#	Article	IF	Citations
127	Supramolecular Assembly of Metal Complexes by (Aryl)Iâ‹…â‹…â‹…d[Pt^{II}] Halogen Bonds. Chemistry - A European Journal, 2020, 26, 7692-7701.	3.3	54
128	Highâ€Level Ab Initio Study of Anionâ€“Ï€ Interactions in Pyridine and Pyrazine Rings Coordinated to Ag^I. ChemPhysChem, 2008, 9, 397-399.	2.1	53
129	Importance of Ï€-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. Crystal Growth and Design, 2019, 19, 5869-5881.	3.0	53
130	Simultaneous Interaction of Tetrafluoroethene with Anions and Hydrogen-Bond Donors: A Cooperativity Study. Journal of Chemical Theory and Computation, 2009, 5, 1186-1194.	5.3	52
131	Energetic vs Synergetic Stability: A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 3266-3273.	2.5	52
132	Anionï¿Ï€ Interactions in Flavoproteins. Chemistry - an Asian Journal, 2011, 6, 2316-2318.	3.3	52
133	Trinuclear and tetranuclear adduct formation between sodium perchlorate and copper(II) complexes of salicylaldimine type ligands: Structural characterization and theoretical investigation. Inorganica Chimica Acta, 2011, 366, 219-226.	2.4	51
134	Differences in Nuclearity, Molecular Shapes, and Coordination Modes of Azide in the Complexes of Cd(II) and Hg(II) with a â€œMetalloligandâ€•[CuL] (H₂L =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 462 Td (N,N Theoretical Calculations. Inorganic Chemistry, 2012, 51, 12407-12418.	4.0	51
135	Ionpair-Ï€ interactions favor cell penetration of arginine/tryptophan-rich cell-penetrating peptides. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183098.	2.6	51
136	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. RSC Advances, 2015, 5, 72923-72936.	3.6	50
137	MP2 Study of Cationâ^'(Ï€)nâ^'Ï€ Interactions (n= 1â^'4). Journal of Physical Chemistry A, 2006, 110, 9307-9309.	2.5	49
138	Crystallographic and Theoretical Evidence of Anionâ€“Ï€ and Hydrogenâ€Bonding Interactions in a Squaramideâ€“Nitrate Salt. European Journal of Organic Chemistry, 2008, 2008, 1864-1868.	2.4	49
139	1,1,2,2-Tetracyanocyclopropane (TCCP) as supramolecular synthon. Physical Chemistry Chemical Physics, 2016, 18, 1693-1698.	2.8	49
140	The development of a promising photosensitive Schottky barrier diode using a novel Cd(<scp>ii</scp>) based coordination polymer. Dalton Transactions, 2017, 46, 13531-13543.	3.3	49
141	Primary Anionâ^'Ï€ Catalysis and Autocatalysis. Journal of the American Chemical Society, 2018, 140, 17867-17871.	13.7	49
142	Anion Recognition by Neutral Chalcogen Bonding Receptors: Experimental and Theoretical Investigations. Chemistry - A European Journal, 2020, 26, 4706-4713.	3.3	49
143	Fluorescent sensing of Al 3+ by benzophenone based Schiff base chemosensor and live cell imaging applications: Impact of keto-enol tautomerism. Sensors and Actuators B: Chemical, 2017, 239, 1194-1204.	7.8	48
144	On the Importance of Ïƒâ€“Hole Interactions in Crystal Structures. Crystals, 2021, 11, 1205.	2.2	48

#	Article	IF	Citations
145	A Theoretical Study of Anionâ€“Ï€ Interactions in Seven-Membered Rings. ChemPhysChem, 2007, 8, 1182-1187.	2.1	47
146	Solvent-driven structural topology involving energetically significant intra- and intermolecular chelate ring contacts and anticancer activities of Cu(<scp>ii</scp>) phenanthroline complexes involving benzoates: experimental and theoretical studies. RSC Advances, 2019, 9, 16339-16356.	3.6	47
147	Energetically significant unconventional Ï€-Ï€ contacts involving fumarate in a novel coordination polymer of Zn(II): In-vitro anticancer evaluation and theoretical studies. Inorganica Chimica Acta, 2019, 493, 1-13.	2.4	47
148	Origin of the regioselective lithiation of 1,3-disubstituted heteroatom aromatics. MNDO evidence for bidentate complexation. Journal of the American Chemical Society, 1992, 114, 9093-9100.	13.7	46
149	Supramolecularly Regulated Ligands for Asymmetric Hydroformylations and Hydrogenations. Chemistry - A European Journal, 2015, 21, 11417-11426.	3.3	46
150	A New Family of Ni₄ and Ni₆ Aggregates from the Self-Assembly of [Ni₂] Building Units: Role of Carboxylate and Carbonate Bridges. Inorganic Chemistry, 2015, 54, 4709-4723.	4.0	46
151	A combined experimental and computational study on supramolecular assemblies in hetero-tetranuclear nickel(<scp>ii</scp>)â€“cadmium(<scp>ii</scp>) complexes with N₂O₄-donor compartmental Schiff bases. Dalton Transactions, 2016, 45, 15048-15059.	3.3	46
152	Anionâ‹…â‹…â‹…Anion Coinage Bonds: The Case of Tetrachloridoaurate. Angewandte Chemie - International Edition, 2021, 60, 14385-14389.	13.8	46
153	Cationic 5-phosphonio-substituted N-heterocyclic carbenes. Dalton Transactions, 2016, 45, 11384-11396.	3.3	45
154	Exploring the coordinative adaptation and molecular shapes of trinuclear CuII2M^{II} (M =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Transactions, 2016, 45, 5730-5740.	3.3	45
155	Self-Assembled Molecular Complexes and Coordination Polymers of Cd^{II}, Hexamine, and Monocarboxylates: Structural Analysis and Theoretical Studies of Supramolecular Interactions. Crystal Growth and Design, 2010, 10, 1677-1687.	3.0	44
156	Non-covalent tetrel bonding interactions in hemidirectional lead(<scp>ii</scp>) complexes with nickel(<scp>ii</scp>)-salen type metalloligands. New Journal of Chemistry, 2018, 42, 6062-6076.	2.8	44
157	Remote Control of Anionâ€“Ï€ Catalysis on Fullereneâ€Centered Catalytic Triads. Angewandte Chemie - International Edition, 2018, 57, 10883-10887.	13.8	44
158	Diaryliodonium as a double Ïƒ-hole donor: the dichotomy of thiocyanate halogen bonding provides divergent solid state arylation by diaryliodonium cations. Organic Chemistry Frontiers, 2020, 7, 2230-2242.	4.5	44
159	Counterintuitive Substituent Effect of the Ethynyl Group in Ionâˆ’Ï€ Interactions. Journal of Physical Chemistry A, 2009, 113, 10367-10375.	2.5	43
160	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
161	Cation-Ï€ vs anion-Ï€ interactions: a complete Ï€-orbital analysis. Chemical Physics Letters, 2004, 399, 220-225.	2.6	42
162	Interplay between cationâ€“Ï€ and hydrogen bonding interactions: Are non-additivity effects additive?. Chemical Physics Letters, 2009, 479, 316-320.	2.6	42

#	Article	IF	Citations
163	Structural characterization, recognition patterns and theoretical calculations of long-chain N-alkyl substituted purine and pyrimidine bases as ligands: On the importance of anionâ€“Ï€ interactions. Coordination Chemistry Reviews, 2013, 257, 2705-2715.	18.8	42
164	Chargeâ€Assisted Chalcogen Bonds: CSD and DFT Analyses and Biological Implication in Glucosidase Inhibitors. Chemistry - A European Journal, 2020, 26, 4599-4606.	3.3	42
165	Anion-Ï€ interactions in five-membered rings: a combined crystallographic and ab initio study. Chemical Physics Letters, 2003, 382, 534-540.	2.6	41
166	Synthesis, structural characterization, theoretical calculations and catecholase mimetic activity of manganese-Schiff base complexes. Polyhedron, 2014, 75, 40-49.	2.2	41
167	Influence of ring size on the strength of carbon bonding complexes between anions and perfluorocycloalkanes. Physical Chemistry Chemical Physics, 2014, 16, 19192-19197.	2.8	41
168	Xâ€ray Crystal Structure of a Metalled Doubleâ€Helix Generated by Infinite and Consecutive C*â€Ag^Iâ€C* (C*:N¹â€Hexylcytosine) Base Pairs through Argentophilic and Hydrogen Bond Interactions. Chemistry - A European Journal, 2017, 23, 2103-2108.	3.3	41
169	Observation of Ï€-hole interactions in the solid state structures of three new copper(II) complexes with a tetradentate N4 donor Schiff base: Exploration of their cytotoxicity against MDA-MB 468 cells. Polyhedron, 2017, 123, 334-343.	2.2	41
170	On the importance of Pbâ‹¯X (X = O, N, S, Br) tetrel bonding interactions in a series of tetra- and hexa-coordinated Pb(<scp>ii</scp>) compounds. CrystEngComm, 2018, 20, 5033-5044.	2.6	41
171	Unexpected chalcogen bonds in tetravalent sulfur compounds. Physical Chemistry Chemical Physics, 2019, 21, 11313-11319.	2.8	41
172	2,5-Furandicarboxylic acid as a linker for lanthanide coordination polymers: the role of heteroaromatic Ï€â€“Ï€ stacking and hydrogen bonding. New Journal of Chemistry, 2019, 43, 2179-2195.	2.8	41
173	Intramolecular Spodium Bonds in Zn(II) Complexes: Insights from Theory and Experiment. International Journal of Molecular Sciences, 2020, 21, 7091.	4.1	41
174	Asymmetric [Nâ€“Iâ€“N]⁺ halonium complexes. Chemical Communications, 2020, 56, 8428-8431.	4.1	41
175	Metal Centers as Nucleophiles: Oxymoron of Halogen Bondâ€Involving Crystal Engineering. Chemistry - A European Journal, 2022, 28, .	3.3	41
176	Metalâ€“organic and supramolecular lead(<scp>ii</scp>) networks assembled from isomeric nicotinoylhydrazone blocks: the effects of ligand geometry and counter-ion on topology and supramolecular assembly. CrystEngComm, 2016, 18, 5375-5385.	2.6	40
177	The role of unconventional stacking interactions in the supramolecular assemblies of Hg(<scp>ii</scp>) coordination compounds. CrystEngComm, 2016, 18, 9056-9066.	2.6	40
178	Synthesis and crystal structures of three new lead(II) isonicotinoylhydrazone derivatives: Anion controlled nuclearity and dimensionality. Inorganica Chimica Acta, 2017, 461, 192-205.	2.4	40
179	Boron triel bonding: a weak electrostatic interaction lacking electron-density descriptors. Physical Chemistry Chemical Physics, 2018, 20, 24192-24200.	2.8	40
180	On the Importance of Pnictogen and Chalcogen Bonding Interactions in Supramolecular Catalysis. International Journal of Molecular Sciences, 2021, 22, 12550.	4.1	40

#	Article	IF	Citations
181	Self-Assembly, Binding, and Dynamic Properties of Heterodimeric Porphyrin Macrocycles. Journal of Organic Chemistry, 2005, 70, 6616-6622.	3.2	39
182	2-Aminopyrimidine Derivatives Exhibiting Anion-Ï€ Interactions: A Combined Crystallographic and Theoretical Study. Crystal Growth and Design, 2009, 9, 2363-2376.	3.0	39
183	Lone pairâ€“Ï€ vs Ï€â€“Ï€ interactions in 5-fluoro-1-hexyluracil and 1-hexyluracil: a combined crystallographic and computational study. CrystEngComm, 2010, 12, 362-365.	2.6	39
184	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
185	Ï€-HoleÂ·Â·Â·d_z²[Pt^{II}] Interactions with Electron-Deficient Arenes Enhance the Phosphorescence of Pt^{II}-Based Luminophores. Inorganic Chemistry, 2020, 59, 9308-9314.	4.0	39
186	Differentiating intramolecular spodium bonds from coordination bonds in two polynuclear zinc(<scp>ii</scp>) Schiff base complexes. CrystEngComm, 2021, 23, 2703-2710.	2.6	39
187	Bifurcated Halogen Bonding Involving Two Rhodium(I) Centers as an Integrated Ï*f*-Hole Acceptor. Jacs Au, 2021, 1, 354-361.	7.9	39
188	Anionâˆ’Ï€ Interactions in Four-Membered Rings. Organic Letters, 2009, 11, 1987-1990.	4.6	38
189	Is the Use of Diffuse Functions Essential for the Properly Description of Noncovalent Interactions Involving Anions?. Journal of Physical Chemistry A, 2013, 117, 2651-2655.	2.5	38
190	Asymmetric Hydrogenation of Sevenâ€Membered C=Nâ€containing Heterocycles and Rationalization of the Enantioselectivity. Chemistry - A European Journal, 2016, 22, 10607-10613.	3.3	38
191	Catecholase activity, DNA binding and cytotoxicity studies of a Cu(<scp>ii</scp>) complex of a pyridoxal schiff base: synthesis, X-ray crystal structure, spectroscopic, electrochemical and theoretical studies. RSC Advances, 2016, 6, 86851-86861.	3.6	38
192	Anionâ€“Ï€ Interactions in Lightâ€Induced Reactions: Role in the Amidation of (Hetero)aromatic Systems with Activated Nâ€Aryloxyamides. Chemistry - A European Journal, 2019, 25, 11785-11790.	3.3	38
193	Semicoordination Bond Breaking and Halogen Bond Making Change the Supramolecular Architecture of Metal-Containing Aggregates. Crystal Growth and Design, 2020, 20, 6956-6965.	3.0	38
194	On the Mechanism of Lithiation of Hydric Aromatics:Â Direct NMR Evidence for Short Hâˆ’Li Contacts in Mixed Aggregates1. Journal of Organic Chemistry, 1996, 61, 5194-5195.	3.2	37
195	Weak Câˆ’H/Ï€ Interaction Participates in the Diastereoselectivity of a Hostâˆ’Guest Complex in the Presence of Six Strong Hydrogen Bonds. Organic Letters, 2003, 5, 1135-1138.	4.6	37
196	Antiproliferative evaluation and supramolecular association in Mn(II) and Zn(II) bipyridine complexes: Combined experimental and theoretical studies. Journal of Inorganic Biochemistry, 2019, 200, 110803.	3.5	37
197	A novel oxalato bridged supramolecular ternary complex of Cu(II) involving energetically significant Ï€-hole interaction: Experimental and theoretical studies. Inorganica Chimica Acta, 2019, 487, 354-361.	2.4	37
198	Interaction of positively and negatively charged aromatic hydrocarbons with benzene and triphenylene: Towards a model of pure organic insulators. Chemical Physics Letters, 2008, 460, 406-410.	2.6	36

#	Article	IF	Citations
199	Observation of novel oxygenâ‹¯oxygen interaction in supramolecular assembly of cobalt(<scp>iii</scp>) Schiff base complexes: a combined experimental and computational study. RSC Advances, 2015, 5, 73028-73039.	3.6	36
200	Synthesis, crystal structure, antimicrobial screening and density functional theory calculation of nickel(II), cobalt(II) and zinc(II) mononuclear Schiff base complexes. Inorganica Chimica Acta, 2015, 425, 211-220.	2.4	36
201	Synthesis, X-ray characterization, DFT calculations and Hirshfeld surface analysis studies of carbohydrazone based on Zn(<scp>ii</scp>) complexes. CrystEngComm, 2016, 18, 102-112.	2.6	36
202	Chelate ring stacking interactions in the supramolecular assemblies of Zn(<scp>ii</scp>)and Cd(<scp>ii</scp>) coordination compounds: a combined experimental and theoretical study. CrystEngComm, 2017, 19, 1389-1399.	2.6	36
203	Energetically favorable anti-electrostatic hydrogen bonded cationic clusters in Ni(II) 3,5-dimethylpyrazole complexes: Anticancer evaluation and theoretical studies. Polyhedron, 2019, 168, 113-126.	2.2	36
204	Supramolecular association in Cu(II) and Co(II) coordination complexes of 3,5-dimethylpyrazole: Experimental and theoretical studies. Inorganica Chimica Acta, 2019, 484, 133-141.	2.4	36
205	Preparation, Solid-State Characterization, and Computational Study of a Crown Ether Attached to a Squaramide. Organic Letters, 2005, 7, 1437-1440.	4.6	35
206	Longâ€Range Effects in Anionâ€“Ï€ Interactions: Their Crucial Role in the Inhibition Mechanism of Mycobacterium Tuberculosis Malate Synthase. Chemistry - A European Journal, 2014, 20, 6985-6990.	3.3	35
207	Sâ‹…â‹…â‹…Sn Tetrel Bonds in the Activation of Peroxisome Proliferatorâ€Activated Receptors (PPARs) by Organotin Molecules. Chemistry - A European Journal, 2018, 24, 16582-16587.	3.3	35
208	Ab initio investigations of lithium diffusion in single-walled carbon nanotubes. Chemical Physics, 2004, 297, 85-91.	1.9	34
209	Design of a dual sensing highly selective cyanide chemodosimeter based on pyridinium ring chemistry. New Journal of Chemistry, 2011, 35, 57-60.	2.8	34
210	Hostâ€“Guest Supramolecular Interactions in the Coordination Compounds of 4,4â€²-Azobis(pyridine) with MnX₂ (X = NCS^{â€“}, NCNCN^{â€“}, and PF₆^{â€“}): Structural Analyses and Theoretical Study. Inorganic Chemistry, 2012, 51, 1837-1851.	4.0	34
211	On the Importance of Unprecedented Lone Pairâ€“Salt Bridge Interactions in Cu(II)â€“Malonateâ€“2-Amino-5-Chloropyridineâ€“Perchlorate Ternary System. Journal of Physical Chemistry A, 2013, 117, 5802-5811.	2.5	34
212	Competition between Halogen Bonding and Ï€â€Hole Interactions Involving Various Donors: The Role of Dispersion Effects. ChemPhysChem, 2015, 16, 3108-3113.	2.1	34
213	Hydrothermal synthesis, X-ray structure and DFT and magnetic studies of a (H₂SiW₁₂O₄₀)^{2â^’} based one-dimensional linear coordination polymer. Dalton Transactions, 2015, 44, 8824-8832.	3.3	34
214	Competition between lone pair-Ï€, halogen-Ï€ and triel bonding interactions involving BX3 (XÂ=ÂF, Cl, Br) Tj ETQq0 0 0 rgBT /Overlock 1	1.4	34
215	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. ChemistrySelect, 2017, 2, 9336-9343.	1.5	34
216	Ï€â€Hole Interactions Involving Nitro Aromatic Ligands in Protein Structures. Chemistry - A European Journal, 2019, 25, 13436-13443.	3.3	34

#	Article	IF	Citations
217	Modulation of coordination in pincer-type isonicotinohydrazone Schiff base ligands by proton transfer. CrystEngComm, 2019, 21, 108-117.	2.6	34
218	Charge-assisted hydrogen bond and nitrileâ‹¯nitrile interaction directed supramolecular associations in Cu(<scp>ii</scp>) and Mn(<scp>ii</scp>) coordination complexes: anticancer, hematotoxicity and theoretical studies. New Journal of Chemistry, 2020, 44, 5473-5488.	2.8	34
219	A novel fluoride selective optical chemosensor based on internal charge transfer signaling. Tetrahedron Letters, 2010, 51, 596-599.	1.4	33
220	Analysis of the contribution of the Ï€-acidity of the s-tetrazine ring in the crystal packing of coordination polymers. CrystEngComm, 2013, 15, 3031.	2.6	33
221	Ïƒ-Hole halogen bonding interactions in a mixed valence cobalt(<scp>iii</scp>/<scp>ii</scp>) complex and anti-electrostatic hydrogen bonding interaction in a cobalt(<scp>iii</scp>) complex: a theoretical insight. CrystEngComm, 2018, 20, 7281-7292.	2.6	33
222	Supramolecular association in Cu(II) coordination complexes involving energetically significant NOâ‹¯NO Ï€â€“hole interaction and cooperative Ï€-stacked ternary assembly: Experimental and theoretical studies. Inorganica Chimica Acta, 2019, 488, 159-169.	2.4	33
223	Spodium bonding in five coordinated Zn(<scp>ii</scp>): a new player in crystal engineering?. CrystEngComm, 2021, 23, 3084-3093.	2.6	33
224	Understanding the Forces That Govern Packing: A Density Functional Theory and Structural Investigation of Anionâ‹¯Ï€â€“Anion and Nonclassical Câ€“HÂ·Â·Â·Anion Interactions. Inorganic Chemistry, 2012, 51, 10334-10340.	4.0	32
225	Feasibility of Single-Walled Carbon Nanotubes as Materials for CO₂ Adsorption: A DFT Study. Journal of Physical Chemistry C, 2012, 116, 21083-21092.	3.1	32
226	Electrostatically enhanced Fâ‹¯F interactions through hydrogen bonding, halogen bonding and metal coordination: an ab initio study. Physical Chemistry Chemical Physics, 2016, 18, 20381-20388.	2.8	32
227	H-Bonded anionâ€“anion complex trapped in a squaramido-based receptor. Chemical Communications, 2018, 54, 1841-1844.	4.1	32
228	A â€œnucleophilicâ€•iodine in a halogen-bonded iodonium complex manifests an unprecedented I+Â·Â·Â·Ag+ interaction. CheM, 2021, 7, 948-958.	11.7	32
229	Theoretical ab initio study of the interplay between hydrogen bonding, cationâ€“Ï€ and Ï€â€“Ï€ interactions. Theoretical Chemistry Accounts, 2009, 122, 325-332.	1.4	31
230	On the Importance of Anionâ€“Ï€ Interactions in the Mechanism of Sulfide:Quinone Oxidoreductase. Chemistry - an Asian Journal, 2013, 8, 2708-2713.	3.3	31
231	Molecular Recognition of Nucleotides in Water by Scorpiandâ€Type Receptors Based on Nucleobase Discrimination. Chemistry - A European Journal, 2014, 20, 3730-3741.	3.3	31
232	Regium-Ï€ vs Cation-Ï€ Interactions in M2 and MCl (M = Cu, Ag and Au) Complexes with Small Aromatic Systems: An ab Initio Study. Inorganics, 2018, 6, 64.	2.7	31
233	Cu(II) and Co(II) coordination solids involving unconventional parallel nitrile(Ï€)â€’nitrile(Ï€) and energetically significant cooperative hydrogen bonding interactions: Experimental and theoretical studies. Journal of Molecular Structure, 2019, 1195, 733-743.	3.6	31
234	Supramolecular network of a framework material supported by the anionâ€“Ï€ linkage of Keggin-type heteropolyoxotungstates: experimental and theoretical insights. Dalton Transactions, 2021, 50, 1895-1900.	3.3	31

#	Article	IF	Citations
235	Direct conversion of white phosphorus to versatile phosphorus transfer reagents via oxidative onioation. Nature Chemistry, 2022, 14, 384-391.	13.6	31
236	Predicting Experimental Complexation-Induced Changes in1H NMR Chemical Shift for Complexes between Zinc-Porphyrins and Amines Using the ab Initio/GIAO-HF Methodology. Organic Letters, 2002, 4, 399-401.	4.6	30
237	Concurrent aerogen bonding and lone pair/anionâ€“Ï€ interactions in the stability of organoxenon derivatives: a combined CSD and ab initio study. Physical Chemistry Chemical Physics, 2017, 19, 30063-30068.	2.8	30
238	Phosphatase Mimicking Activity of Two Zinc(II) Schiff Base Complexes with Zn₂O₂ÂCores: NBO Analysis and MEP Calculation to Estimate Nonâ€Covalent Interactions. ChemistrySelect, 2017, 2, 6286-6295.	1.5	30
239	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
240	Remote Control of Anionâ€“Ï€ Catalysis on Fullereneâ€Centered Catalytic Triads. Angewandte Chemie, 2018, 130, 11049-11053.	2.0	30
241	Formation of a tetranuclear supramolecule via non-covalent Pbâ‹¯Cl tetrel bonding interaction in a hemidirected lead(<scp>ii</scp>) complex with a nickel(<scp>ii</scp>) containing metaloligand. CrystEngComm, 2019, 21, 6859-6868.	2.6	30
242	Supramolecular association involving nitrileâ€“nitrile interactions in polymeric Mn(II) coordination complexes: A combined experimental and theoretical study. Inorganica Chimica Acta, 2019, 487, 424-432.	2.4	30
243	One-Pot Route to X-perfluoroarenes (X = Br, I) Based on Fe^{III}-Assisted Câ€“F Functionalization and Utilization of These Arenes as Building Blocks for Crystal Engineering Involving Halogen Bonding. Crystal Growth and Design, 2020, 20, 5908-5921.	3.0	30
244	Dual Cation and Anion Acceptor Molecules. The Case of the (Î·6-C6H6)(Î·6C6F6)Cr(0) Complex. Journal of Physical Chemistry A, 2007, 111, 3137-3142.	2.5	29
245	A Combined Experimental and Theoretical Study of Anionâ€“Ï€ Interactions in Bis(pyrÂimidine) Salts. European Journal of Organic Chemistry, 2007, 2007, 5821-5825.	2.4	29
246	MP2 study of anionâ€“Ï€ complexes of trifluoro-s-triazine with tetrahedral and octahedral anions. Chemical Physics Letters, 2007, 438, 104-108.	2.6	29
247	A combined experimental and computational study of supramolecular assemblies in ternary copper(<scp>ii</scp>) complexes with a tetradentate N₄donor Schiff base and halides. RSC Advances, 2014, 4, 58643-58651.	3.6	29
248	Synthesis, Structure, and Binding Properties of Lipophilic Cavitands Based on a Calix[4]pyrrole-Resorcinarene Hybrid Scaffold. Journal of Organic Chemistry, 2014, 79, 5545-5557.	3.2	29
249	Combined Experimental and Theoretical Investigation of Ligand and Anion Controlled Complex Formation with Unprecedented Structural Features and Photoluminescence Properties of Zinc(II) Complexes. Crystal Growth and Design, 2014, 14, 4111-4123.	3.0	29
250	From monomers to polymers: steric and supramolecular effects on dimensionality of coordination architectures of heteroleptic mercury(<scp>ii</scp>) halogenideâ€“tetradentate Schiff base complexes. CrystEngComm, 2015, 17, 3493-3502.	2.6	29
251	Solvent-Triggered Cis/Trans Isomerism in Cobalt Dioxolene Chemistry: Distinguishing Effects of Packing on Valence Tautomerism. Inorganic Chemistry, 2016, 55, 8331-8340.	4.0	29
252	Synthesis, X-ray characterization, DFT calculations and Hirshfeld surface analysis of thiosemicarbazone complexes of Mⁿ⁺ ions (n = 2, 3; M = Ni, Cd, Mn, Co and Cu). CrystEngComm, 2016, 18, 1009-1023.	2.6	29

#	Article	IF	Citations
253	One pot synthesis of two cobalt(<scp>iii</scp>) Schiff base complexes with chelating pyridyltetrazolate and exploration of their bio-relevant catalytic activities. RSC Advances, 2018, 8, 28216-28237.	3.6	29
254	Magnetic, luminescence, topological and theoretical studies of structurally diverse supramolecular lanthanide coordination polymers with flexible glutaric acid as a linker. New Journal of Chemistry, 2019, 43, 14546-14564.	2.8	29
255	Diastereoselective Amplification of a Mechanically Chiral [2]Catenane. Journal of the American Chemical Society, 2021, 143, 11957-11962.	13.7	29
256	On the Importance of Halogen Bonding Interactions in Two X-ray Structures Containing All Four (F,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	2.2	29
257	Substituent effects in cationâ€“Ï€ interactions revisited: a general approach based on intrinsic properties of the arenes. Physical Chemistry Chemical Physics, 2014, 16, 1322-1326.	2.8	28
258	Triple-bridged ferromagnetic nickel(ii) complexes: A combined experimental and theoretical DFT study on stabilization and magnetic coupling. Dalton Transactions, 2014, 43, 6455.	3.3	28
259	Role of ligand backbone of tridentate Schiff-base on complex nuclearity and bio-relevant catalytic activities of zinc(II) complexes: Experimental and theoretical investigations. Inorganica Chimica Acta, 2014, 421, 364-373.	2.4	28
260	On the Versatility of BH₂X (X=F, Cl, Br, and I) Compounds as Halogenâ€, Hydrogenâ€, and Trielâ€Bond Donors: An Abâ€...Initio Study. ChemPhysChem, 2016, 17, 3181-3186.	2.1	28
261	Ligandâ€Flexibility Controlled and Solventâ€Induced Nuclearity Conversion in Cu^{II}â€Based Catecholase Models: A Deep Insight Through Combined Experimental and Theoretical Investigations. European Journal of Inorganic Chemistry, 2017, 2017, 133-145.	2.0	28
262	Formation of a water-mediated assembly of two neutral copper(<scp>ii</scp>) Schiff base fragments with a Cu₂(NCS)₄moiety: exploration of non-covalent Câ€“Hâ‹¯Ï€(bimetallo ring) interactions. CrystEngComm, 2018, 20, 1679-1689.	2.6	28
263	Werner type clathrates involving guest benzoic acid and benzoate in discrete Mn(II) hosts: Experimental and theoretical studies. Polyhedron, 2019, 159, 387-399.	2.2	28
264	Engineering Crystals Using sp 3 â€C Centred Tetrel Bonding Interactions. Chemistry - A European Journal, 2020, 26, 10126-10132.	3.3	28
265	Synthesis, X-ray characterization and regium bonding interactions of a trichlorido(1-hexylcytosine)gold(<scp>iii</scp>) complex. Chemical Communications, 2020, 56, 3524-3527.	4.1	28
266	Predicting Directed Lithiations by Means of MNDO-Determined Agostic Interaction Parameters and Proximity Features. Peri Lithiation of Polyhydric Phenolic Compounds. Journal of the American Chemical Society, 1995, 117, 1105-1116.	13.7	28
267	Cisâ€“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. Dalton Transactions, 2012, 41, 12200.	3.3	27
268	Estimating ring strain energies in small carbocycles by means of the Baderâ€™s theory of â€˜atoms-in-moleculesâ€™. Chemical Physics Letters, 2012, 536, 165-169.	2.6	27
269	Synthesis, X-ray characterization, DFT calculations and Hirshfeld surface analysis of Zn(<scp>ii</scp>) and Cd(<scp>ii</scp>) complexes based on isonicotinoylhydrazone ligand. CrystEngComm, 2016, 18, 4587-4596.	2.6	27
270	On the importance of antiparallel C Oâ‹¯Câ€“F interactions in N1-(3-hydroxypropyl)-5-fluorouracilateâ€“Hg(II) complex: A combined X-ray and DFT study. Inorganica Chimica Acta, 2016, 452, 244-250.	2.4	27

#	Article	IF	Citations
271	Methylene spacer regulated variation in conformation of tetradentate N₂O₂ donor Schiff bases trapped in manganese(<scp>iii</scp>) complexes. CrystEngComm, 2018, 20, 1077-1086.	2.6	27
272	Adipato bridged novel hexanuclear Cu(<scp>ii</scp>) and polymeric Co(<scp>ii</scp>) coordination compounds involving cooperative supramolecular assemblies and encapsulated guest water clusters in a square grid host: antiproliferative evaluation and theoretical studies. Dalton Transactions, 2020, 49, 9863-9881.	3.3	27
273	Recurrent Supramolecular Motifs in a Series of Acidâ€“Base Adducts Based on Pyridine-2,5-Dicarboxylic Acid N-Oxide and Organic Bases: Inter- and Intramolecular Hydrogen Bonding. Crystal Growth and Design, 2020, 20, 1738-1751.	3.0	27
274	Seâ‹…â‹…â‹…O/S and Sâ‹…â‹…â‹…â‹…O Chalcogen Bonds in Small Molecules and Proteins: A Combined CSD and PDB Study. ChemBioChem, 2022, 23, e202100498.	2.6	27
275	RI-MP2 and MPWB1K Study of Ï€â€“Anionâˆ™Ï€â€² Complexes: MPWB1K Performance and Some Additivity Aspects. Journal of Chemical Theory and Computation, 2011, 7, 3012-3018.	5.3	26
276	Polymorphism in hetero-metallic tri-nuclear CuII2CdII complexes of salicylaldimine ligand: Structural analysis and theoretical study. Polyhedron, 2013, 52, 1416-1424.	2.2	26
277	Surprising behaviour of Mâ€“CO(lone pair)â‹¯Ï€(arene) interactions in the solid state of fluorinated oxaphosphirane complexes. CrystEngComm, 2015, 17, 1769-1772.	2.6	26
278	Experimental observation and theoretical investigation of a novel Cd(<scp>ii</scp>) complex with Ï€-hole interactions involving nitro groups. CrystEngComm, 2015, 17, 3912-3916.	2.6	26
279	Tetranuclear manganese(II) complexes of hydrazone and carbohydrazone ligands: Synthesis, crystal structures, magnetic properties, Hirshfeld surface analysis and DFT calculations. Inorganica Chimica Acta, 2016, 443, 101-109.	2.4	26
280	Supramolecular nanotubes based on halogen bonding interactions: cooperativity and interaction with small guests. Physical Chemistry Chemical Physics, 2017, 19, 12936-12941.	2.8	26
281	Exploration of photocatalytic activity of an end-on azide bridged one-dimensional cadmium(II) Schiff base complex for the degradation of organic dye in visible light. Polyhedron, 2017, 121, 199-205.	2.2	26
282	Enhanced Photosensitive Schottky Diode Behavior of Pyrazine over 2-Aminopyrimidine Ligand in Copper(II)-Phthalate MOFs: Experimental and Theoretical Rationalization. ACS Omega, 2018, 3, 9160-9171.	3.5	26
283	H-Bonded anionâ€“anion complexes in fentanyl citrate polymorphs and solvates. Chemical Communications, 2019, 55, 115-118.	4.1	26
284	Energetically significant antiparallel Ï€-stacking contacts in Co(II), Ni(II) and Cu(II) coordination compounds of pyridine-2,6-dicarboxylates: Antiproliferative evaluation and theoretical studies. Inorganica Chimica Acta, 2020, 501, 119233.	2.4	26
285	Favipiravir: insight into the crystal structure, Hirshfeld surface analysis and computational study. Journal of the Iranian Chemical Society, 2022, 19, 85-94.	2.2	26
286	OPLS allâ€atom force field for carbohydrates. Journal of Computational Chemistry, 1997, 18, 1955-1970.	3.3	26
287	Synthesis, crystal structure, magnetic property and DFT calculations of an unusual dinuclear Î¼2-alkoxido bridged iron(iii) complex. Dalton Transactions, 2013, 42, 12274.	3.3	25
288	Influence of accompanying anions on supramolecular assembly and coordination geometry in HgII complexes with 8-aminoquinoline: experimental and theoretical studies. CrystEngComm, 2013, 15, 1404.	2.6	25

#	Article	IF	Citations
289	Supramolecular architecture constructed from the hemidirected lead(II) complex with N'-(4-hydroxybenzylidene)isonicotinohydrazide. Inorganica Chimica Acta, 2020, 502, 119350.	2.4	25
290	Regiumâ^Ï€ Bonds Are Involved in Proteinâ€“Gold Binding. Journal of Physical Chemistry Letters, 2020, 11, 8259-8263.	4.6	25
291	Tetrel Bonding and Other Non-Covalent Interactions Assisted Supramolecular Aggregation in a New Pb(II) Complex of an Isonicotinohydrazide. Molecules, 2020, 25, 4056.	3.8	25
292	Halogen Bonds in Protein Nucleic Acid Recognition. Journal of Chemical Theory and Computation, 2020, 16, 4744-4752.	5.3	25
293	Synthesis of Ni(<scp>ii</scp>)â€“Mn(<scp>ii</scp>) complexes using a new mononuclear Ni(<scp>ii</scp>) complex of an unsymmetrical N₂O₃ donor ligand: structures, magnetic properties and catalytic oxidase activity. Dalton Transactions, 2021, 50, 4686-4699.	3.3	25
294	Spodium bonding and other non-covalent interactions assisted supramolecular aggregation in a new mercury(II) complex of a nicotinohydrazide derivative. Inorganica Chimica Acta, 2021, 519, 120279.	2.4	25
295	Electron belt-to-Ïƒ-hole switch of noncovalently bound iodine(<scp>i</scp>) atoms in dithiocarbamate metal complexes. Inorganic Chemistry Frontiers, 2021, 8, 2505-2517.	6.0	25
296	On the importance of Ï€-hole spodium bonding in tricoordinated Hg^{II}complexes. Dalton Transactions, 2020, 49, 17547-17551.	3.3	25
297	Synthesis, spectroscopic findings and crystal engineering of Pb(<scp>ii</scp>)â€“Salen coordination polymers, and supramolecular architectures engineered by Ïƒ-hole/spodium/tetrel bonds: a combined experimental and theoretical investigation. RSC Advances, 2022, 12, 6352-6363.	3.6	25
298	Ab initio investigations of lithium insertion in boron and nitrogen-doped single-walled carbon nanotubes. Chemical Physics Letters, 2005, 411, 256-261.	2.6	24
299	Synthesis, X-ray structure analysis and computational studies of novel bis(thiocarbamoyl) disulfides with non-covalent Sâ‹¯N and Sâ‹¯S interactions. Chemical Physics Letters, 2006, 422, 234-239.	2.6	24
300	Interplay between Edge-to-Face Aromatic and Hydrogen-Bonding Interactions. Journal of Physical Chemistry A, 2008, 112, 6017-6022.	2.5	24
301	Synthesis and Crystal Structures of Î¼â€Oxidoâ€•and Î¼â€Hydroxidoâ€Bridged Dinuclear Iron(III) Complexes with an N₂O Donor Ligand â€“ A Theoretical Study on the Influence of Weak Forces on the Feâ€“Oâ€“Fe Bridging Angle. European Journal of Inorganic Chemistry, 2011, 2011, 2558-2566.	2.0	24
302	Experimental and Theoretical Study of Aromaticity Effects in the Solid State Architecture on Squaric Acid Derivatives. Crystal Growth and Design, 2014, 14, 2578-2587.	3.0	24
303	Enantiopure bisphosphine ligands with appended crown ether groups as regulation sites for Rh-mediated hydrogenations. Tetrahedron, 2015, 71, 4490-4494.	1.9	24
304	Inorganicâ€“organic hybrid materials based on PbBr₂and pyridineâ€“hydrazone blocks â€“ structural and theoretical study. RSC Advances, 2016, 6, 60385-60393.	3.6	24
305	Unveiling the effects of the in situ generated arene anion radical and imine radical on catecholase like activity: a DFT supported experimental investigation. Dalton Transactions, 2017, 46, 5888-5900.	3.3	24
306	Hydrogen- and halogen-bond cooperativity in determining the crystal packing of dihalogen charge-transfer adducts: a study case from heterocyclic pentatomic chalcogenone donors. CrystEngComm, 2017, 19, 4401-4412.	2.6	24

#	Article	IF	Citations
307	Structures, photoresponse properties and DNA binding abilities of 4-(4-pyridinyl)-2-pyridone salts. RSC Advances, 2019, 9, 9663-9677.	3.6	24
308	Unconventional DNA-relevant Ï€-stacked hydrogen bonded arrays involving supramolecular guest benzoate dimers and cooperative anionâ€“Ï€/Ï€â€“Ï€/Ï€â€“anion contacts in coordination compounds of Co(<scp>ii</scp>) and Zn(<scp>ii</scp>) phenanthroline: experimental and theoretical studies. New Journal of Chemistry, 2020, 44, 4504-4518.	2.8	24
309	Bifurcated Î¼₂-IÂ·Â·Â·(N,O) Halogen Bonding: The Case of (Nitrosoguanidinate)Ni^{II} Cocrystals with Iodine(I)-Based Ïƒ-Hole Donors. Crystal Growth and Design, 2021, 21, 588-596.	3.0	24
310	Utility of Three-Coordinate Silver Complexes Toward the Formation of Iodonium Ions. Inorganic Chemistry, 2021, 60, 5383-5390.	4.0	24
311	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
312	Unexpected Nonadditivity Effects in Anionâˆ’Ï€ Complexes. Journal of Physical Chemistry A, 2011, 115, 7849-7857.	2.5	23
313	A methodological analysis for the assessment of non-covalent Ï€ interactions. Chemical Physics Letters, 2011, 508, 144-148.	2.6	23
314	Two mixed-ligand cadmium(<scp>ii</scp>) 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
315	Valence tautomerism induced nucleophilic ipso substitution in a coordinated tetrabromocatecholate ligand and diverse catalytic activity mimicking the function of phenoxazinone synthase. Journal of Molecular Catalysis A, 2016, 412, 56-66.	4.8	23
316	A highly selective â€œONâ€“OFFâ€•probe for colorimetric and fluorometric sensing of Cu²⁺ in water. RSC Advances, 2017, 7, 11312-11321.	3.6	23
317	Cooperative influence of pseudohalides and ligand backbone of Schiff-bases on nuclearity and stereochemistry of cobalt(<scp>iii</scp>) complexes: experimental and theoretical investigation. Dalton Transactions, 2017, 46, 15257-15268.	3.3	23
318	Molecular electrostatic potential and â€œatomsâ€•inâ€•moleculesâ€•analyses of the interplay between Ï€â€•hole and lone pairÂ·Â·Â·Ï€/Xâ€“HÂ·Â·Â·Ï€/metalÂ·Â·Â·Ï€ interactions. Journal of Computational Chemistry, 2018, 39, 458-463.	3.3	23
319	Halogen bonding effects on the outcome of reactions at metal centres. Chemical Communications, 2019, 55, 2380-2383.	4.1	23
320	On the importance of antiparallel Ï€â€“Ï€ interactions in the solid state of isatin-based hydrazides. New Journal of Chemistry, 2019, 43, 8122-8131.	2.8	23
321	Synchronized On/Off Switching of Four Binding Sites for Water in a Molecular Solomon Link. Angewandte Chemie - International Edition, 2019, 58, 8053-8057.	13.8	23
322	Energetically significant unconventional O Hâ‹¯Ï€ contacts involving discrete guest (H2O)8 clusters in a fumarato bridged polymeric supramolecular host of Ni(II) phenanthroline: Antiproliferative evaluation and theoretical studies. Polyhedron, 2020, 176, 114266.	2.2	23
323	Reaction of Cu(II) Chelates with Uranyl Nitrate to Form a Coordination Complex or H-Bonded Adduct: Experimental Observations and Rationalization by Theoretical Calculations. Inorganic Chemistry, 2020, 59, 15848-15861.	4.0	23
324	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. New Journal of Chemistry, 2020, 44, 19541-19554.	2.8	23

#	Article	IF	Citations
325	Diaryliodonium Tetrachloroplatinates(II): Recognition of a Trifurcated Metal-Involving Î¼₃-lÂ·Â·Â·(Cl,Cl,Pt) Halogen Bond. Crystal Growth and Design, 2021, 21, 5360-5372.	3.0	23
326	Substituent Effects in Ionâˆ’Ï€ Interactions: Fine-Tuning via the Ethynyl Group. Journal of Physical Chemistry A, 2010, 114, 1926-1930.	2.5	22
327	A combined experimental and theoretical study of the supramolecular self-assembly of Cu(II) malonate complex assisted by various weak forces and water dimer. Journal of Solid State Chemistry, 2014, 220, 149-156.	2.9	22
328	Theoretical study on Ïƒ- and Ï€-hole carbonâ‹¯carbon bonding interactions: implications in CFC chemistry. Physical Chemistry Chemical Physics, 2016, 18, 32155-32159.	2.8	22
329	Chalcogen â€¯like-likeâ€™ Interactions Involving Trisulphide and Triselenide Compounds: A Combined CSD and Ab Initio Study. Molecules, 2018, 23, 699.	3.8	22
330	Theoretical and Crystallographic Study of Lead(IV) Tetrel Bonding Interactions. Chemistry - A European Journal, 2019, 25, 6007-6013.	3.3	22
331	Diethylaminophenyl-based Schiff base Cu(<scp>ii</scp>) and V(<scp>iv</scp>) complexes: experimental and theoretical studies and cytotoxicity assays. New Journal of Chemistry, 2019, 43, 18832-18842.	2.8	22
332	Supramolecular assembly of a 2D coordination polymer bearing pyridine-N-oxide-2,5-dicarboxylic acid and copper ion: X-ray crystallography and DFT calculations. Journal of Molecular Structure, 2020, 1202, 127243.	3.6	22
333	Oxalato bridged coordination polymer of manganese(<scp>iii</scp>) involving unconventional Oâ‹¯Ï€-hole(nitrile) and antiparallel nitrileâ‹¯nitrile contacts: antiproliferative evaluation and theoretical studies. New Journal of Chemistry, 2020, 44, 20021-20038.	2.8	22
334	Covalent and Non-covalent Noble Gas Bonding Interactions in XeFn Derivatives (n = 2â€“6): A Combined Theoretical and ICSD Analysis. Frontiers in Chemistry, 2020, 8, 395.	3.6	22
335	Supramolecular and theoretical perspectives of 2,2â€²:6â€²,2â€²â€²-terpyridine based Ni(<scp>ii</scp>) and Cu(<scp>ii</scp>) complexes: on the importance of Câ€“Hâ‹¯Cl and Ï€â‹¯Ï€ interactions. New Journal of Chemistry, 2020, 44, 7310-7318.	2.8	22
336	X-ray characterization, Hirshfeld surface analysis, DFT calculations,in vitroandin silicolipoxygenase inhibition (LOX) studies of dichlorophenyl substituted 3-hydroxy-chromenones. New Journal of Chemistry, 2021, 45, 19928-19940.	2.8	22
337	Theoretical and Crystallographic Study of the Dual Ïƒ/Ï€ Anion Binding Affinity of Quinolizinylium Cation. Journal of Chemical Theory and Computation, 2008, 4, 1981-1989.	5.3	21
338	Theoretical and crystallographic study of edge-to-face aromatic interactions between pyridine moieties and benzene. Chemical Physics Letters, 2009, 468, 280-285.	2.6	21
339	A polynuclear and two dinuclear copper(II) Schiff base complexes: Synthesis, characterization, self-assembly, magnetic property and DFT study. Polyhedron, 2017, 137, 332-346.	2.2	21
340	Multicomponent Supramolecular Assemblies of Melamine and Î±-Hydroxycarboxylic Acids: Understanding the Hydrogen Bonding Patterns and Their Physicochemical Consequences. Crystal Growth and Design, 2018, 18, 6786-6800.	3.0	21
341	Methylene spacer regulated variation in molecular and crystalline architectures of cobalt(<scp>iii</scp>) complexes with reduced Schiff base ligands: a combined experimental and theoretical study. Dalton Transactions, 2019, 48, 11433-11447.	3.3	21
342	Theoretical ab Initio Study on Cooperativity Effects between Nitro Ï€â€hole and Halogen Bonding Interactions. ChemPhysChem, 2019, 20, 1135-1144.	2.1	21

#	Article	IF	Citations
343	Supramolecular assemblies involving salt bridges: DFT and X-ray evidence of bipolarity. CrystEngComm, 2020, 22, 8171-8181.	2.6	21
344	A new spodium bond driven coordination polymer constructed from mercury(<scp>ii</scp>) azide and 1,2-bis(pyridin-2-ylmethylene)hydrazine. New Journal of Chemistry, 2020, 44, 21100-21107.	2.8	21
345	Noble Gas Bonding Interactions Involving Xenon Oxides and Fluorides. Molecules, 2020, 25, 3419.	3.8	21
346	Spodium Bonds: Noncovalent Interactions Involving Groupâ€...12 Elements. Angewandte Chemie, 2020, 132, 17635-17640.	2.0	21
347	Charge assisted halogen and pnictogen bonds: insights from the Cambridge Structural Database and DFT calculations. CrystEngComm, 2020, 22, 7162-7169.	2.6	21
348	Biological promiscuity of a binuclear Cu(<scp>ii</scp>) complex of aminoguanidine Schiff base: DNA binding, anticancer activity and histidine sensing ability of the complex. New Journal of Chemistry, 2020, 44, 7319-7328.	2.8	21
349	Crystal engineering with pyrazolyl-thiazole derivatives: structure-directing role of Ï€-stacking and Ïƒ-hole interactions. CrystEngComm, 2021, 23, 3276-3287.	2.6	21
350	Spodium Bonds in Biological Systems: Expanding the Role of Zn in Protein Structure and Function. Journal of Chemical Information and Modeling, 2021, 61, 3945-3954.	5.4	21
351	Noncovalent Interactions Involving Group 6â€‰in Biological Systems: The Case of Molybdopterin and Tungstopterin Cofactors. Chemistry - A European Journal, 2022, 28, .	3.3	21
352	Induced-Polarization Energy Map:â€‰ A Helpful Tool for Predicting Geometric Features of Anion-Ï€ Complexes. Journal of Chemical Theory and Computation, 2007, 3, 2098-2107.	5.3	20
353	Erroneous behaviour of the widely used MP2(full)/aug-cc-pVXZ (X=D,T) level of theory for evaluating the BSSE in ionâ€“Ï€ complexes. Chemical Physics Letters, 2010, 489, 254-258.	2.6	20
354	Tuning of the anionâ€“Ï€ interaction. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	20
355	Synthesis, structure and DFT study of a chelidamic acid based Cu coordination polymer: On the importance of Ï€â€“Ï€ interactions and hexameric water clusters. Journal of Molecular Structure, 2015, 1080, 30-36.	3.6	20
356	Auxiliary Part of Ligand Mediated Unique Coordination Chemistry of Copper (II). ChemistrySelect, 2016, 1, 615-625.	1.5	20
357	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
358	A novel method for copper(<scp>ii</scp>) mediated region-selective bromination of aromatic rings under mild conditions. RSC Advances, 2016, 6, 61214-61220.	3.6	20
359	Design of end-on cyanato bridged trinuclear Cu(II) Schiff base complex with salen type Schiff base ligand: synthesis, structural investigation and DFT study. Journal of Coordination Chemistry, 2017, 70, 1389-1405.	2.2	20
360	Anion-reliant structural versatility of novel cadmium(II) complexes: Synthesis, crystal structures, photoluminescence properties and exploration of unusual OÂ·Â·Â·S chalcogen bonding involving thiocyanate coligand. Inorganica Chimica Acta, 2018, 469, 189-196.	2.4	20

#	Article	IF	Citations
361	Lone pairâ€“Ï€vs.Ïƒ-holeâ€“Ï€ interactions in bromine head-containing oxacalix[2]arene[2]triazines. CrystEngComm, 2018, 20, 3251-3257.	2.6	20
362	Formation of an imidazoliumyl-substituted [(L_C)₄P₄]⁴⁺tetracation and transition metal mediated fragmentation and insertion reaction (L_C= NHC). Chemical Science, 2019, 10, 6868-6875.	7.4	20
363	Unconventional formation of a 1D-chain of H-bonded water molecules in bipyridine-based supramolecular hexameric hosts of isostructural coordination compounds of Co(II) and Zn(II): Antiproliferative evaluation and theoretical studies. Polyhedron, 2020, 191, 114809.	2.2	20
364	Electrophilic behaviour of 3-methyl-2-methylthio-1,3,4-thiadiazolium salts: A multimodal theoretical approach. Arkivoc, 2005, 2005, 415-437.	0.5	20
365	Anionâ€“Ï€ Catalysis Enabled by the Mechanical Bond**. Angewandte Chemie - International Edition, 2022, 61, .	13.8	20
366	Structural and energetic features of single-walled carbon nanotube junctions: a theoretical ab initio study. Chemical Physics, 2004, 303, 265-270.	1.9	19
367	A Combined Experimental and Theoretical Study of Anionâ€“Ï€ Interactions inN⁶â€• andN⁹â€Decyladenine Salts. European Journal of Organic Chemistry, 2010, 2010, 5171-5180.	2.4	19
368	Influence of para substituents in controlling photophysical behavior and different non-covalent weak interactions in zinc complexes of a phenol based â€œend-offâ€•compartmental ligand. Dalton Transactions, 2015, 44, 20032-20044.	3.3	19
369	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
370	On the Importance of Ï€â€Hole Beryllium Bonds: Theoretical Study and Biological Implications. Chemistry - A European Journal, 2017, 23, 5375-5380.	3.3	19
371	A versatile chemosensor for the detection of Al³⁺ and picric acid (PA) in aqueous solution. Dalton Transactions, 2018, 47, 15907-15916.	3.3	19
372	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. CrystEngComm, 2018, 20, 6490-6501.	2.6	19
373	Intramolecular Noncovalent Carbon Bonding Interaction Stabilizes the cis Conformation in Acylhydrazones. ChemPlusChem, 2018, 83, 881-885.	2.8	19
374	Two Geometrical Isomers of a 1D Coordination Polymer: Rationalization by Theoretical Calculations and Variation of Electrical Properties with the Change in Binding Mode of Dicarboxylate Linker. Crystal Growth and Design, 2019, 19, 5819-5828.	3.0	19
375	Nitropyridine-1-Oxides as Excellent Ï€-Hole Donors: Interplay between Ïƒ-Hole (Halogen, Hydrogen, Triel,) Tj ETQq1 1 0.784314 rgBT /O 20, 3440.	4.1	19
376	Photosensitive Schottky barrier diode behavior of a semiconducting Co(<scp>iii</scp>)â€“Na complex with a compartmental Schiff base ligand. RSC Advances, 2019, 9, 34710-34719.	3.6	19
377	Stabilization of two conformers via intra- or inter-molecular hydrogen bonds in a dinuclear vanadium(<scp>v</scp>) complex with a pendant Schiff base: theoretical insight. RSC Advances, 2019, 9, 35165-35175.	3.6	19
378	The Effect of Guest Metal Ions on the Reduction Potentials of Uranium(VI) Complexes: Experimental and Theoretical Investigations. Chemistry - A European Journal, 2020, 26, 1612-1623.	3.3	19

#	Article	IF	Citations
379	DFT Analysis of Uncommon Ï€Â·Â·Â·H-Bond Array Interaction in a New Pterostilbene/Theophylline Cocrystal. Crystal Growth and Design, 2020, 20, 6691-6698.	3.0	19
380	Recurrent motifs in pharmaceutical cocrystals involving glycolic acid: X-ray characterization, Hirshfeld surface analysis and DFT calculations. CrystEngComm, 2020, 22, 6674-6689.	2.6	19
381	Self-assembly hexanuclear metallacontainer hosting halogenated guest species and sustaining structure of 3D coordination framework. Chemical Communications, 2011, 47, 1764-1766.	4.1	18
382	Dinuclear and heptanuclear nickel(II) complexes: Anion coordination induced ligand arm hydrolysis and aggregation around a nickel(II) core. Polyhedron, 2013, 53, 32-39.	2.2	18
383	Synthesis, X-ray characterization and DFT studies of bis-N-imidazolylpyrimidine salts: the prominent role of hydrogen bonding and anionâ€“Ï€ interactions. CrystEngComm, 2014, 16, 9043-9053.	2.6	18
384	Cadmium(<scp>ii</scp>) complexes containing N,Nâ€²-dimethylviolurate as ligand or counteranion: synthesis, characterization, crystal structures and DFT study. RSC Advances, 2015, 5, 10826-10836.	3.6	18
385	Synthesis, X-ray characterization and DFT studies of N-benzimidazolyl-pyrimidineâ€“M(<scp>ii</scp>) complexes (M = Cu, Co and Ni): the prominent role of Ï€-hole and anionâ€“Ï€ interactions. CrystEngComm, 2015, 17, 5987-5997.	2.6	18
386	Self-assembly synthesis, structure, topology, and magnetic properties of a mononuclear Fe(<scp>iii</scp>)-violurate derivative: a combined experimental and theoretical study. Dalton Transactions, 2016, 45, 16166-16172.	3.3	18
387	Structural diversity and non-covalent interactions in Cd(II) and Zn(II) complexes derived from 3,5-dinitrobenzoic acid and pyridine: Experimental and theoretical aspects. Inorganica Chimica Acta, 2016, 440, 38-47.	2.4	18
388	Dangling and Hydrolyzed Ligand Arms in [Mn3] and [Mn6] Coordination Assemblies: Synthesis, Characterization, and Functional Activity. Inorganic Chemistry, 2017, 56, 2639-2652.	4.0	18
389	Synthesis, Characterization, DFT Study, Catechol Oxidase and Phenoxazinone Synthase Like Activities of Two New Manganese(IV) Schiff Base Complexes. ChemistrySelect, 2017, 2, 2975-2984.	1.5	18
390	The first X-ray structure of a silverâ€“nucleotide complex: interaction of ion Ag(<scp>i</scp>) with cytidine-5â€²-monophosphate. CrystEngComm, 2017, 19, 5830-5834.	2.6	18
391	Accidental Orthogonality Induced Weak Magnetic Coupling in a Dinuclear Copper(II) Complex: Exploration of Unconventional Câ€¢Hâ‹…â‹…â‹…Ï€(SCN) Interactions and Catechol Oxidase Activity. ChemistrySelect, 2017, 2, 6535-6543.	1.5	18
392	Valenceâ€Tautomerismâ€Driven Aromatic Nucleophilic Substitution in Cobaltâ€Bound Tetrabromocatecholate Ligands â€“ Influence of Positive Charge at the Ligand Backbone on Phenoxazinone Synthase Activity. European Journal of Inorganic Chemistry, 2018, 2018, 924-931.	2.0	18
393	Bipolar behaviour of salt-bridges: a combined theoretical and crystallographic study. New Journal of Chemistry, 2018, 42, 12134-12142.	2.8	18
394	Indirect influence of alkyl substituent on sigma-hole interactions: The case study of antimony(III) diphenyldithiophosphates with covalent Sb-S and non-covalent Sbâ‹¯S pnictogen bonds. Polyhedron, 2019, 173, 114126.	2.2	18
395	â€œLikeâ€“likeâ€•tetrel bonding interactions between Sn centres: a combinedab initioand CSD study. Dalton Transactions, 2019, 48, 11208-11216.	3.3	18
396	Analysis of energies of halogen and hydrogen bonding interactions in the solid state structures of vanadyl Schiff base complexes. RSC Advances, 2019, 9, 4789-4796.	3.6	18

#	Article	IF	Citations
397	Quantifying Intramolecular Halogen Bonds in Nucleic Acids: A Combined Protein Data Bank and Theoretical Study. ACS Chemical Biology, 2020, 15, 1942-1948.	3.4	18
398	Exploration of Brâ‹¯O halogen bonding interactions in dinuclear vanadium(V) complexes with Schiff base ligands. Polyhedron, 2020, 187, 114676.	2.2	18
399	Experimental and theoretical study of thymine and cytosine derivatives: the crucial role of weak noncovalent interactions. CrystEngComm, 2012, 14, 5777.	2.6	17
400	Theoretical ab initio study of anionâ€“Ï€ interactions in inorganic rings. Chemical Physics Letters, 2012, 530, 145-150.	2.6	17
401	Anionâ€“Ï€ interactions in [S4N3]+ rings. New Journal of Chemistry, 2013, 37, 2636.	2.8	17
402	On the Importance of Cï£¿H/Ï€ and Cï£¿Hâ‹…â‹…â‹…Hï£¿C Interactions in the Solid State Structure of 15â€Lipoxygenase Inhibitors Based on Eugenol Derivatives. ChemPhysChem, 2015, 16, 2260-2266.	2.1	17
403	The N-atom in [N(PR₃)₂]⁺ cations (R = Ph, Me) can act as electron donor for (pseudo) anti-electrostatic interactions. CrystEngComm, 2015, 17, 3768-3771.	2.6	17
404	Synthesis, structure, magnetic property and self-assembly of two double end-on azide bridged ferromagnetic nickel(II) complexes with distinct bidentate blocking ligands: A combined experimental and theoretical study. Polyhedron, 2015, 101, 257-269.	2.2	17
405	Carbodiphosphorane mediated synthesis of a triflyloxyphosphonium dication and its reactivity towards nucleophiles. Chemical Communications, 2017, 53, 2954-2957.	4.1	17
406	New pyridoxal based chemosensor for selective detection of Zn2+: Application in live cell imaging and phosphatase activity response. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 334, 86-100.	3.9	17
407	On the Importance of Halogenâ€“Halogen Interactions in the Solid State of Fullerene Halides: A Combined Theoretical and Crystallographic Study. Crystals, 2017, 7, 191.	2.2	17
408	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
409	A versatile quinoxaline derivative serves as a colorimetric sensor for strongly acidic pH. Dalton Transactions, 2018, 47, 17077-17085.	3.3	17
410	Coordination Polymers Based on Phthalic Acid and Aminopyrazine Ligands: On the Importance of Nâ€“HÂ·Â·Â·Ï€ Interactions. Polymers, 2018, 10, 182.	4.5	17
411	Supramolecular association involving antiparallel COâ‹¯CO and anionâ€“Ï€ contacts in Co(II) and Mn(II) complexes involving 2,5-pyridinedicarboxylate: Anticancer evaluation and theoretical studies. Inorganica Chimica Acta, 2019, 498, 119108.	2.4	17
412	Energetically significant cooperative Ï€-stacked ternary assemblies in Ni(II) phenanthroline compounds involving discrete water clusters: Anticancer activities and theoretical studies. Journal of Molecular Structure, 2021, 1229, 129486.	3.6	17
413	Cd(II) coordination polymer of fumaric acid and pyridyl-hydrazide Schiff base: Structure, photoconductivity and theoretical interpretation. Inorganica Chimica Acta, 2021, 518, 120253.	2.4	17
414	Coordinationversusspodium bonds in dinuclear Zn(<scp>ii</scp>) and Cd(<scp>ii</scp>) complexes with a dithiophosphate ligand. New Journal of Chemistry, 2021, 45, 19402-19415.	2.8	17

#	Article	IF	Citations
415	Syntheses, crystal structures and supramolecular assemblies of two Cu(<scp>ii</scp>) complexes based on a new heterocyclic ligand: insights into Câ€“Hâ‹¯Cl and Ï€â‹¯Ï€ interactions. CrystEngComm, 2022, 24, 1598-1611.	2.6	17
416	RNAs' uracil quartet model with a non-essential metal ion. Chemical Communications, 2011, 47, 4646.	4.1	16
417	Metallomacrocycles as anion receptors: combining hydrogen bonding and ion pair based hosts formed from Ag(i) salts and flexible bis- and tris-pyrimidine ligands. Chemical Communications, 2013, 49, 4944.	4.1	16
418	Two new copper and nickel complexes of pyridine-2,6-dicarboxylic acid N-oxide and their proton transferred salts: Solid state and DFT insights. Inorganica Chimica Acta, 2015, 438, 135-145.	2.4	16
419	Synthesis, X-ray characterization and DFT study of a novel Fe(III)â€“pyridine-2,6-dicarboxylic acid N-oxide complex with unusual coordination mode. Inorganica Chimica Acta, 2016, 449, 44-51.	2.4	16
420	Importance of chelateâ€“chelate stacking interactions in crystal structures of square pyramidal copper(II) complexes with two distinct chelating bidentate ligands. Inorganica Chimica Acta, 2016, 442, 16-23.	2.4	16
421	Importance of Câ€“Hâ‹¯Ï€ interactions in stabilizing the syn/anti arrangement of pendant alkoxy side arms in two manganese(<scp>iv</scp>) Schiff base complexes: exploration of catechol oxidase and phenoxazinone synthase like activities. New Journal of Chemistry, 2017, 41, 8053-8065.	2.8	16
422	Suitable Interplay between Various Conventional and Unconventional Nonâ€Covalent Interactions in Forming Selfâ€Assembled Supramolecules of Two Ni(II)/Zn(II) Schiff Base Complexes. ChemistrySelect, 2017, 2, 7880-7887.	1.5	16
423	A Combined Experimental and Theoretical Study to Explore the Importance of Ïƒâ€Hole Carbon Bonding Interactions in Stabilizing Molecular Assemblies. ChemistrySelect, 2017, 2, 10586-10594.	1.5	16
424	Intramolecular Ï€â€“hole interactions with nitro aromatics. CrystEngComm, 2019, 21, 5410-5417.	2.6	16
425	Adenine as a Halogen Bond Acceptor: A Combined Experimental and DFT Study. Crystals, 2019, 9, 224.	2.2	16
426	Structures, Photoresponse Properties, and Biological Activity of Dicyano-Substituted 4-Aryl-2-pyridone Derivatives. ACS Omega, 2019, 4, 7200-7212.	3.5	16
427	Self-assembly of amphiphilic aryl-squaramides in water driven by dipolar Ï€â€“Ï€ interactions. Organic and Biomolecular Chemistry, 2020, 18, 888-894.	2.8	16
428	Energetically significant anti-parallel Ï€-stacking and unconventional anion-Ï€ interactions in phenanthroline based Ni(II) and Cu(II) coordination compounds: Antiproliferative evaluation and theoretical studies. Inorganica Chimica Acta, 2021, 516, 120082.	2.4	16
429	Iodonium complexes of the tertiary amines quinuclidine and 1-ethylpiperidine. Dalton Transactions, 2021, 50, 8297-8301.	3.3	16
430	Zwitterionic iodonium species afford halogen bond-based porous organic frameworks. Chemical Science, 2022, 13, 5650-5658.	7.4	16
431	Towards Anion Recognition and Precipitation with Water-Soluble 1,2,4-Selenodiazolium Salts: Combined Structural and Theoretical Study. International Journal of Molecular Sciences, 2022, 23, 6372.	4.1	16
432	The resonance model in amides: a combined crystallographic and ab initio investigation. New Journal of Chemistry, 2001, 25, 259-261.	2.8	15

#	Article	IF	Citations
433	A combined experimental and theoretical study on supramolecular assemblies in octahedral cobalt(III) salicylaldimine complexes having pendant side arms. Polyhedron, 2016, 112, 86-95.	2.2	15
434	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
435	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
436	Structure guided or structure guiding? Mixed carbon/hydrogen bonding in a bis-Schiff base of N-allyl isatin. CrystEngComm, 2018, 20, 150-154.	2.6	15
437	Surface-grafted lanthanoid complexes of the tungstosilicate polyanion [SiW₁₂O₄₀]^{4â^'}: a synthetic, structural and computational investigation. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 1300-1309.	0.5	15
438	Effects of N-oxidation on the molecular and crystal structures and properties of isocinchomeronic acid, its metal complexes and their supramolecular architectures: experimental, CSD survey, solution and theoretical approaches. RSC Advances, 2019, 9, 25382-25404.	3.6	15
439	A combined experimental and theoretical analysis of the solid-state supramolecular self-assembly of N-(2,4-dichlorophenyl)-1-naphthamide: Synthesis, anticholinesterase potential and molecular docking analysis. Journal of Molecular Structure, 2019, 1197, 458-470.	3.6	15
440	Supramolecular Assemblies in Pb(II) Complexes with Hydrazido-Based Ligands. Crystals, 2019, 9, 323.	2.2	15
441	Antiproliferative evaluation and supramolecular association involving electrostatically enhanced Ï€-Ï€ interaction in isostructural coordination solids of Mn(II), Co(II) and Zn(II) chlorobenzoates: Experimental and theoretical studies. Inorganica Chimica Acta, 2019, 498, 119161.	2.4	15
442	Tetranuclear Mn^{II}/Zn^{II} and Novel Azidoâ€Bridged Chairâ€Shaped Heptanuclear Cd^{II} Compounds: The Effect of Metal Ion and Coordination Mode of the Azide Group on the Structure of the Products. European Journal of Inorganic Chemistry, 2019, 2019, 262-270.	2.0	15
443	Seven and eight-coordinate Fe(III) complexes containing pre-organized ligand 1,10-phenanthroline-2,9-dicarboxylic acid: Solvent effects, supramolecular interactions and DFT calculations. Inorganica Chimica Acta, 2019, 484, 264-275.	2.4	15
444	Methylene spacer regulated variation in supramolecular assembly of zinc(<scp>ii</scp>) dicyanamide complexes with reduced Schiff base ligands: synthesis, structure and DFT study. CrystEngComm, 2020, 22, 6876-6885.	2.6	15
445	Sildenafilâ€“Resorcinol Cocrystal: XRPD Structure and DFT Calculations. Crystals, 2020, 10, 1126.	2.2	15
446	Relevant Ï€-hole tetrel bonding interactions in ethyl 2-triazolyl-2-oxoacetate derivatives: Hirshfeld surface analysis and DFT calculations. CrystEngComm, 2020, 22, 3567-3578.	2.6	15
447	Highly polar stacking interactions wrap inorganics in organics: lone-pairâ€“Ï€-hole interactions between the PdO₄ core and electron-deficient arenes. Inorganic Chemistry Frontiers, 2021, 8, 4965-4975.	6.0	15
448	On the energetic stability of halogen bonds involving metals: implications in crystal engineering. CrystEngComm, 2022, 24, 4440-4446.	2.6	15
449	Solid-State Redox Chemistry: Preparation of 1,4-Naphthoquinone, Hydroquinone, and the Corresponding Mixed Quinhydrone in the Solid State. Journal of Chemical Education, 1995, 72, 63.	2.3	14
450	Ab initio calculations on zinc porphyrins complexed to amines: geometrical details and NMR chemical shifts. Computational and Theoretical Chemistry, 2000, 531, 381-386.	1.5	14

#	Article	IF	Citations
451	Counterintuitive affinity of [2.2]paracyclophane to cations. Chemical Physics Letters, 2005, 408, 59-64.	2.6	14
452	Can lone pair-Ï€ and cation-Ï€ interactions coexist? A theoretical study. Open Chemistry, 2011, 9, 25-34.	1.9	14
453	Isolation of Azadiphosphiridines and Diphosphenimines by Cycloaddition of Azides and a Cationic Diphosphene. Angewandte Chemie - International Edition, 2017, 56, 6218-6222.	13.8	14
454	EPR interpretation, magnetism and biological study of a Cu(II) dinuclear complex assisted by a schiff base precursor. Journal of Biological Inorganic Chemistry, 2017, 22, 481-495.	2.6	14
455	Solid-state inclusion of C₆₀ and C₇₀ in a co-polymer induced by metalâ€“ligand coordination of a Znâ€“porphyrin cage with a bis-pyridyl perylene derivative. CrystEngComm, 2017, 19, 4911-4919.	2.6	14
456	Polymorphism in secondary squaramides: on the importance of Ï€-interactions involving the four membered ring. CrystEngComm, 2018, 20, 237-244.	2.6	14
457	Adsorption and Quantification of Volatile Organic Compounds (VOCs) by using Hybrid Magnetic Nanoparticles. Chemistry - A European Journal, 2018, 24, 12820-12826.	3.3	14
458	A theoretical insight into non-covalent supramolecular interactions in the solid state structures of two octahedral iron(<scp>iii</scp>) complexes. CrystEngComm, 2020, 22, 5731-5742.	2.6	14
459	Magnetically separable nanocatalyst (IL@CuFe2O4-L-Tyr-TiO2/TiTCIL): Preparation, characterization and its applications in 1,2,3-triazole synthesis and in photodegradation of MB. Journal of Molecular Structure, 2021, 1224, 129029.	3.6	14
460	Ï€-Hole spodium bonding in tri-coordinated Hg(<scp>ii</scp>) complexes. Dalton Transactions, 2021, 50, 7545-7553.	3.3	14
461	Selenium chalcogen bonds are involved in proteinâ€“carbohydrate recognition: a combined PDB and theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 17656-17662.	2.8	14
462	Biologically relevant unusual cooperative assemblies and fascinating infinite crown-like supramolecular nitrateâ€“water hosts involving guest complex cations in bipyridine and phenanthroline-based Cu(<scp>ii</scp>) coordination compounds: antiproliferative evaluation and theoretical studies. New Journal of Chemistry, 2021, 45, 8269-8282.	2.8	14
463	On the importance of the inclusion of the basis set superposition error counterpoise correction during optimization of ion-Ï€ complexes. Chemical Physics Letters, 2008, 455, 325-330.	2.6	13
464	Cooperativity effects between non-covalent interactions: Are they important for Z-DNA stability?. Chemical Physics Letters, 2010, 485, 221-225.	2.6	13
465	Radical cation (CË™+â€“Ï€) and radical anion (AË™â¯â€“Ï€) interactions with aromatic rings: energetic, orbitalic and spin density considerations. Physical Chemistry Chemical Physics, 2011, 13, 16698.	2.8	13
466	Effect of a methyl group on the spontaneous resolution of a square-pyramidal coordination compound: crystal packing and conglomerate formation. CrystEngComm, 2012, 14, 5854.	2.6	13
467	Self-assembly cavitand precisely recognizing hexafluorosilicate: a concerted action of two coordination and twelve CHâ‹¯F bonds. Chemical Communications, 2013, 49, 9018.	4.1	13
468	Reversible switching of the electronic ground state in a pentacoordinated Cu(ii) complex. Chemical Communications, 2013, 49, 7806.	4.1	13

#	Article	IF	Citations
469	A dodecanuclear copper(<scp>ii</scp>) cage self-assembled from six dicopper building units. Dalton Transactions, 2014, 43, 4076-4085.	3.3	13
470	Two types of nitrito support for Î¼₄-oxido-bridged [Cu₄] complexes: synthesis, crystal structures, magnetic properties and DFT analysis. Dalton Transactions, 2015, 44, 6107-6117.	3.3	13
471	Experimental and theoretical study of weak intermolecular interactions in crystalline tertiary squaramides. CrystEngComm, 2016, 18, 6437-6443.	2.6	13
472	Exploration of unconventional Ï€â€“hole and Câ€“Hâ‹¯Hâ€“C types of supramolecular interactions in a trinuclear Cd(<scp>ii</scp>) and a heteronuclear Cd(<scp>ii</scp>)â€“Ni(<scp>ii</scp>) complex and experimental evidence for preferential site selection of the ligand by 3d and 4d metal ions. RSC Advances, 2016, 6, 39376-39386.	3.6	13
473	Carboxylate Coordination Assisted Aggregation for Quasiâ€Tetrahedral and Partialâ€Dicubane [Cu₄] Coordination Clusters. ChemistrySelect, 2016, 1, 64-75.	1.5	13
474	The Mouse in a Trap: Observation of a C(sp3)â€“FÂ·Â·Â·Fâ€“C(sp3) Interaction in a Discrete CFC Pair by the Crystal Sponge Method. Crystal Growth and Design, 2017, 17, 3611-3615.	3.0	13
475	The crucial role of chelate-chelate stacking interactions in the crystal structure of a square planar copper(II) complex. Journal of Molecular Structure, 2017, 1127, 355-360.	3.6	13
476	closo-Carboranes as dual CHâ‹¯Ï€ and BHâ‹¯Ï€ donors: theoretical study and biological significance. Physical Chemistry Chemical Physics, 2019, 21, 19944-19950.	2.8	13
477	Crystal structures of N6-modified-amino acid related nucleobase analogs (II): hybrid adenine-Î²-alanine and adenine-GABA molecules. New Journal of Chemistry, 2019, 43, 9680-9688.	2.8	13
478	A triple alkoxo bridged dinuclear cobalt(III) complex mimicking phosphatase and showing ability to degrade organic dye contaminants by photocatalysis. Journal of Organometallic Chemistry, 2019, 883, 52-64.	1.8	13
479	Interconvertible Hydrochlorothiazideâ€“Caffeine Multicomponent Pharmaceutical Materials: A Solvent Issue. Crystals, 2020, 10, 1088.	2.2	13
480	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. Polyhedron, 2020, 187, 114629.	2.2	13
481	A series of hydrogen bond mediated dinuclear nickel(II) complexes with reduced Schiff base ligands: An insight into the nature of their short intermolecular hydrogen bonds. Polyhedron, 2020, 179, 114374.	2.2	13
482	Energetically significant nitrileâ‹¯nitrile and unconventional Câ€“Hâ‹¯Ï€(nitrile) interactions in pyridine based Ni(II) and Zn(II) coordination compounds: Antiproliferative evaluation and theoretical studies. Journal of Molecular Structure, 2021, 1223, 129246.	3.6	13
483	A tetrameric uudd 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. Inorganica Chimica Acta, 2021, 515, 120057.	2.4	13
484	Synthesis and characterization of a mononuclear zinc(<scp>ii</scp>) Schiff base complex: on the importance of Câ€“Hâ‹¯Ï€ interactions. RSC Advances, 2021, 11, 30148-30155.	3.6	13
485	Biologically relevant and energetically significant cooperative ternary (Ï€â€“Ï€)2/(Ï€â€“Ï€)1/(Ï€â€“Ï€)2 assemblies and fascinating discrete (H2O)21 clusters in isostructural 2,5-pyridine dicarboxylato Co(ii) and Zn(ii) phenanthroline compounds: antiproliferative evaluation and theoretical studies. New Journal of Chemistry, 2021, 45, 3699-3715.	2.8	13
486	Nickel(<scp>ii</scp>) complexes based on dithiolateâ€“polyamine binary ligand systems: crystal structures, hirshfeld surface analysis, theoretical study, and catalytic activity study on photocatalytic hydrogen generation. Dalton Transactions, 2021, 50, 5632-5643.	3.3	13

#	Article	IF	Citations
487	Nucleophilic iodonium interactions (NIIs) in 2-coordinate iodine(<scp>i</scp>) and silver(<scp>i</scp>) complexes. Chemical Communications, 2021, 57, 5094-5097.	4.1	13
488	Synthesis, characterization, DNA binding ability, in vitro cytotoxicity, electrochemical properties and theoretical studies of copper(II) carboxylate complexes. Inorganica Chimica Acta, 2021, 518, 120235.	2.4	13
489	Charge Assisted S/Se Chalcogen Bonds in SAM Riboswitches: A Combined PDB and ab Initio Study. ACS Chemical Biology, 2021, 16, 1701-1708.	3.4	13
490	Synthesis and crystal structure of the simultaneous binding of Ni(<scp>ii</scp>) cation and chloride by the protonated 2,4,6 tris-(2-pyridyl)-1,3,5 triazine ligand: theoretical investigations of anionâ‹Ï€, Ï€â‹Ï€ and hydrogen bonding interactions. New Journal of Chemistry, 2021, 45, 11689-11696.	2.8	13
491	The role of Ï€â€“Ï€ stacking and hydrogen-bonding interactions in the assembly of a series of isostructural group IIB coordination compounds. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 178-188.	0.5	13
492	Chameleonic metal-bound isocyanides: a Ï€-donating Cu^I-center imparts nucleophilicity to the isocyanide carbon toward halogen bonding. Inorganic Chemistry Frontiers, 2022, 9, 1655-1665.	6.0	13
493	Metal Coordination Enhances Chalcogen Bonds: CSD Survey and Theoretical Calculations. International Journal of Molecular Sciences, 2022, 23, 4188.	4.1	13
494	Double group-transfer reactions: a theoretical (AM1) approach. Journal of Organic Chemistry, 1992, 57, 6731-6735.	3.2	12
495	OPLS all-atom force field for squaramides and squaric acid. Chemical Physics Letters, 2001, 350, 331-338.	2.6	12
496	A theoretical ab initio study of [n.n]paracyclophane complexes with cations. Chemical Physics Letters, 2006, 417, 371-377.	2.6	12
497	MP2 Study of the Dual Ïƒ/Ï€â^'Anion-Binding Affinity of Fluorinated Phthallic Acid Anhydrides. Journal of Physical Chemistry A, 2008, 112, 1622-1626.	2.5	12
498	Interplay between ionâ€“Ï€ and Ar/Ï€ Van der Waals interactions. Computational and Theoretical Chemistry, 2012, 998, 51-56.	2.5	12
499	Experimental and theoretical studies on the coordination chemistry of the N1-hexyl substituted pyrimidines (uracil, 5-fluorouracil and cytosine). Dalton Transactions, 2013, 42, 7631.	3.3	12
500	Syntheses, crystal structures and density functional theory investigations of copper(<scp>ii</scp>) complexes bearing tridentate Schiff base ligands derived from 8-aminoquinoline. CrystEngComm, 2015, 17, 5664-5671.	2.6	12
501	Synthesis, Structures, and DFT Study of CuBr Based Coordination Polymers via in Situ Reduction of Copper(II). Crystal Growth and Design, 2015, 15, 257-267.	3.0	12
502	Supramolecular interactions through lone pair(lp)â€“Ï€ and hydrogen bonding in cobalt(III) and manganese(II) derivatives of N,Nâ€²-dimethylvioluric acid: A combined experimental and theoretical study. Inorganica Chimica Acta, 2015, 435, 178-186.	2.4	12
503	Anion dependent supramolecular architectures in Cu(II) complexes containing N2O-donor Schiff-base and 4,4â€²-bipyridine ligands: Structural analyses and theoretical studies. Inorganica Chimica Acta, 2016, 448, 26-33.	2.4	12
504	Molecular and crystalline architectures based on HgI₂: from metallamacrocycles to coordination polymers. CrystEngComm, 2017, 19, 3322-3330.	2.6	12

#	Article	IF	Citations
505	Selective and Reversible Fluoride Complexation from Water by a Cyclic Tri(phosphonio)methanide Dication. Angewandte Chemie - International Edition, 2017, 56, 7907-7911.	13.8	12
506	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. Journal of Molecular Structure, 2017, 1141, 225-236.	3.6	12
507	Anionâ^Ï€ Interactions in Hollow Crystals of a Copper(II)-Cyamelurate Coordination Complex. Crystal Growth and Design, 2018, 18, 2636-2644.	3.0	12
508	A comparative experimental and theoretical investigation of hydrogen-bond, halogen-bond and Ï€â€“Ï€ interactions in the solid-state supramolecular assembly of 2- and 4-formylphenyl arylsulfonates. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 816-829.	0.5	12
509	Hydrogen Bond versus Halogen Bond in HXOn (X = F, Cl, Br, and I) Complexes with Lewis Bases. Inorganics, 2019, 7, 9.	2.7	12
510	Synthesis, Xâ€ray characterization and density functional theory studies of N⁶â€benzylâ€N⁶â€methyladenineâ€“M(II) complexes (MÂ=ÂZn, Cd): The prominent role of Ï€â€“Ï€, Câ€“HÂ·Â·Â·Ï€ and anionâ€“Ï€ interactions. Applied Organometallic Chemistry, 2019, 33, e4906.	3.8	12
511	An inorganicâ€“organic hybrid supramolecular framework based on the Î³-[Mo₈O₂₆]^{4â^'} cluster and cobalt complex of aspartic acid: X-ray structure and DFT study. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 469-477.	0.5	12
512	Diverse structural assemblies of U-shaped hydrazinyl-sulfonamides: experimental and theoretical analysis of non-covalent interactions stabilizing solid state conformations. CrystEngComm, 2019, 21, 1780-1793.	2.6	12
513	Tetrel Bonding Interactions Involving Carbon at Work: Recent Advances in Crystal Engineering and Catalysis. Journal of Carbon Research, 2020, 6, 60.	2.7	12
514	A facile biomimetic catalytic activity through hydrogen atom abstraction by the secondary coordination sphere in manganese(<scp>iii</scp>) complexes. Dalton Transactions, 2020, 49, 14216-14230.	3.3	12
515	Halogenâ‹¯halogen interactions in decahalo-closo-carboranes: CSD analysis and theoretical study. Physical Chemistry Chemical Physics, 2020, 22, 6122-6130.	2.8	12
516	Theoretical study of spodium bonding in the active site of three Zn-proteins and several model systems. Physical Chemistry Chemical Physics, 2021, 23, 16888-16896.	2.8	12
517	A theoretical insight into the formation of chalcogen bonding (ChB) interactions involving coordinated DMSO molecules as Ïƒ-hole donors and benzoate groups as Ïƒ-hole acceptors in a dinuclear copper(<scp>ii</scp>) complex. CrystEngComm, 2021, 23, 5087-5096.	2.6	12
518	Solvothermal self assembly of three lanthanide(III)-succinates: Crystal structure, topological analysis and DFT calculations on water channel. Journal of Molecular Structure, 2021, 1245, 131094.	3.6	12
519	Macrocyclic complexes based on [Nâ‹¯Iâ‹¯N]⁺ halogen bonds. Chemical Communications, 2021, 57, 12464-12467.	4.1	12
520	Complexes of Zinc(II) with Nâ€imidazolylâ€and Nâ€Pyrazolylpyrimidine Donor Ligands: Synthesis, Crystal Structures, and Theoretical Study. European Journal of Inorganic Chemistry, 2012, 2012, 3995-4003.	2.0	11
521	Anionâ€“Ï€ Interactions Involving [MX_n]^{mâ^'} Anions: A Comprehensive Theoretical Study. ChemPhysChem, 2013, 14, 145-154.	2.1	11
522	On the nature of Mâ€“CO(lone pair)â‹¯Ï€(arene) interactions in the solid state of fluorinated oxaphosphirane complexes. CrystEngComm, 2015, 17, 6736-6743.	2.6	11

#	Article	IF	Citations
523	A combined experimental and theoretical study on two new dinuclear cadmium(II) Schiff base complexes with selenocyanate-Î²-Se. Inorganica Chimica Acta, 2016, 453, 51-61.	2.4	11
524	Unraveling the dual character of sulfur atoms in a series of Hg(<scp>ii</scp>) coordination polymers containing bis(4-pyridyl)disulfide. CrystEngComm, 2017, 19, 1974-1981.	2.6	11
525	Synthesis and supramolecular self-assembly of thioxothiazolidinone derivatives driven by H-bonding and diverse Ï€â€“hole interactions: A combined experimental and theoretical analysis. Journal of Molecular Structure, 2017, 1139, 209-221.	3.6	11
526	Both end-on and end-to-end azide bridged tetranuclear ferromagnetic nickel(<scp>ii</scp>) Schiff base complexes. New Journal of Chemistry, 2017, 41, 13585-13592.	2.8	11
527	Estimation of non-covalent C Hâ‹¯Ï€, Ï€â‹¯Ï€ (chelate ring) and hydrogen bonding interactions in vanadium(V) Schiff base complexes: Methylene spacer regulated variation in self-assembly. Inorganica Chimica Acta, 2017, 467, 212-220.	2.4	11
528	Synthesis, Substitution, and Oxidation of Imidazoleâ€2â€thione Based Tricyclic 1,4â€Dihydroâ€1,4â€diphosphinines. European Journal of Inorganic Chemistry, 2018, 2018, 904-916.	2.0	11
529	Tetrel Bonding Interactions in Perchlorinated Cyclopenta- and Cyclohexatetrelanes: A Combined DFT and CSD Study. Molecules, 2018, 23, 1770.	3.8	11
530	Effect of temperature and ligand protonation on the electronic ground state in Cu(<scp>ii</scp>) polymers having unusual secondary interactions: a magnetic and catechol oxidase study. Dalton Transactions, 2018, 47, 16102-16118.	3.3	11
531	Substituent Effects in Multivalent Halogen Bonding Complexes: A Combined Theoretical and Crystallographic Study. Molecules, 2018, 23, 18.	3.8	11
532	Synthesis, structure, physicochemical characterization and theoretical evaluation of non-covalent interaction energy of a polymeric copper(II)-hydrazone complex. Inorganica Chimica Acta, 2019, 484, 95-103.	2.4	11
533	Observation of an anionâ‹¯anion interaction in a square planar copper(II) Schiff base complex: DFT study and CSD analysis. Inorganica Chimica Acta, 2019, 487, 465-472.	2.4	11
534	Synthesis, characterization and DFT study on two copper(II) complexes with a naphthalene-based Schiff base: Examples of stronger chelateâ€“chelate interactions than those reported for classical Ï€â€“Ï€ complexes. Polyhedron, 2019, 157, 487-494.	2.2	11
535	A theoretical insight on the anionâ‹¯anion interactions observed in the solid state structure of a hetero-trinuclear complex. CrystEngComm, 2021, 23, 1429-1438.	2.6	11
536	A new coordination polymer constructed from Pb(NO3)2 and a benzylideneisonicotinohydrazide derivative: Coordination-induced generation of a Ï€-hole towards a tetrel-bonding stabilized structure. Journal of Molecular Structure, 2021, 1234, 130139.	3.6	11
537	Hydrogen bond mediated intermolecular magnetic coupling in mononuclear high spin iron(<scp>iii</scp>) Schiff base complexes: synthesis, structure and magnetic study with theoretical insight. RSC Advances, 2021, 11, 3315-3323.	3.6	11
538	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
539	Structural basis for molecular recognition, theoretical studies andÂanti-bacterial properties of three bis-uracil derivatives. Tetrahedron, 2014, 70, 6931-6937.	1.9	10
540	Unveiling NO2Ï€Â·Â·Â·CC Ï€â€“hole interactions: A combined computational and crystallographic study. Chemical Physics Letters, 2015, 633, 282-286.	2.6	10

#	Article	IF	Citations
541	Electronic Structure of N₂P₂ Four-Membered Rings and the Effect of Their Ligand Coordination to M(CO)₅ (Cr, Mo, and W). Organometallics, 2015, 34, 355-360.	2.3	10
542	Reconciling Experiment and Theory in the Use of Aryl-Extended Calix[4]pyrrole Receptors for the Experimental Quantification of Chlorideâ€“Ï€ Interactions in Solution. International Journal of Molecular Sciences, 2015, 16, 8934-8948.	4.1	10
543	A combined experimental and computational study of supramolecular assemblies in two photoluminescent cadmium(II) complexes with halosalicylaldimine Schiff bases. Inorganica Chimica Acta, 2016, 450, 321-329.	2.4	10
544	Synthesis and Investigation of Solid- and Solution-State Structures of Nickel(II) Complexes with 1,3-Dimethyl-5-(arylazo)-6-aminouracil. European Journal of Inorganic Chemistry, 2016, 2016, 5585-5593.	2.0	10
545	Melamine-mediated self-assembly of a Cu(II)â€“methylmalonate complex assisted by Ï€⁺â€“Ï€⁺ and anti-electrostatic H-bonding interactions. Journal of Coordination Chemistry, 2017, 70, 463-474.	2.2	10
546	Nuclearity versus oxidation state in the catalytic efficiency of Mn^{II/III}azo Schiff base complexes: computational study on supramolecular interactions and phenoxazinone synthase-like activity. New Journal of Chemistry, 2017, 41, 11607-11618.	2.8	10
547	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. Inorganica Chimica Acta, 2018, 482, 384-394.	2.4	10
548	Influence of the aromatic surface on the capacity of adsorption of VOCs by magnetite supported organicâ€“inorganic hybrids. RSC Advances, 2019, 9, 24184-24191.	3.6	10
549	Gallic Acid Dimer As a Double Ï€â€“Hole Donor: Evidence from X-ray, Theoretical Calculations, and Generalization from the Cambridge Structural Database. Crystal Growth and Design, 2019, 19, 3989-3997.	3.0	10
550	Controlled scrambling reactions to polyphosphanes via bond metathesis reactions. Chemical Science, 2019, 10, 11054-11063.	7.4	10
551	On the supramolecular properties of neutral, anionic and cationic cadmium complexes harvested from dithiolateâ€“polyamine binary ligand systems. CrystEngComm, 2020, 22, 8023-8035.	2.6	10
552	Radicalâ‹¯radical chalcogen bonds: CSD analysis and DFT calculations. Physical Chemistry Chemical Physics, 2020, 22, 12757-12765.	2.8	10
553	A late appearing polymorph of nutraceutical pterostilbene. CrystEngComm, 2020, 22, 4680-4684.	2.6	10
554	Diminishing accessibility of electrophilic nickel(<scp>ii</scp>) centres due to incorporation of a methylene spacer in the pendant side arm of a series of heterotrinuclear nickel(<scp>ii</scp>)/sodium complexes: a DFT study using a homodesmotic equation. CrystEngComm, 2020, 22, 2970-2977.	2.6	10
555	Two new hydrogen-bonded supramolecular dioxo-molybdenum(VI) complexes based on acetyl-hydrazone ligands: Synthesis, crystal structure and DFT studies. Journal of Molecular Structure, 2021, 1226, 129346.	3.6	10
556	Biological halogen bonds in proteinâ€“ligand complexes: a combined QTAIM and NCIPlot study in four representative cases. Organic and Biomolecular Chemistry, 2021, 19, 6858-6864.	2.8	10
557	Noble metals in polyoxometalates. Inorganica Chimica Acta, 2021, 523, 120410.	2.4	10
558	Unconventional Ï€-hole and Semi-coordination regium bonding interactions directed supramolecular assemblies in pyridinedicarboxylato bridged polymeric Cu(II) Compounds: Antiproliferative evaluation and theoretical studies. Inorganica Chimica Acta, 2021, 525, 120461.	2.4	10

#	Article	IF	Citations
559	Phenanthroline-based Ni(II) coordination compounds involving unconventional discrete fumarate-water-nitrate clusters and energetically significant cooperative ternary Ï€-stacked assemblies: Antiproliferative evaluation and theoretical studies. Journal of Molecular Structure, 2022, 1248, 131424.	3.6	10
560	Solvothermal synthesis and crystal structures of two Holmium(III)-5-Hydroxyisophthalate entangled coordination polymers and theoretical studies on the importance of Ï€â€¢â€¢â€¢Ï€ stacking interactions. Journal of Molecular Structure, 2022, 1254, 132329.	3.6	10
561	Topochemical [2 + 2] Cycloaddition in a Two-Dimensional Metalâ€“Organic Framework via SCSC Transformation Impacts Halogen‹b›Â·Â·Â·‹/b›Halogen Interactions. Inorganic Chemistry, 2022, 61, 3029-3032.	4.0	10
562	Insight into charge transportation in cadmium based semiconducting organicâ€“inorganic hybrid materials and their application in the fabrication of photosensitive Schottky devices. Dalton Transactions, 2022, 51, 5721-5734.	3.3	10
563	Anion-Responsive Fluorescent Supramolecular Gels. Molecules, 2022, 27, 1257.	3.8	10
564	Polymorphism in the 1/1 Pterostilbene/Picolinic Acid Cocrystal. Crystal Growth and Design, 2022, 22, 590-597.	3.0	10
565	Squaramido-based receptors: applicability of molecular interaction potential to molecular recognition of polyalkylammonium compounds. Theoretical Chemistry Accounts, 2000, 104, 50-66.	1.4	9
566	A topological analysis of charge density in complexes between derivatives of squaric acid and ammonium cation. Chemical Physics Letters, 2001, 339, 369-374.	2.6	9
567	Relevant and unprecedented Câ€“H/Ïƒ supramolecular interactions involving Ïƒ-aromatic M‹sub›2‹/sub›X‹sub›2‹/sub› cores. Dalton Transactions, 2014, 43, 6195-6211.	3.3	9
568	Modulation in Ï€â‹¯Ï€, cationâ‹¯Ï€ and Câ€“Hâ‹¯Hâ€“C interactions varying the counter anions in square planar nickel(II) Schiff base complexes: A combined experimental and theoretical study. Polyhedron, 2016, 119, 451-459.	2.2	9
569	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
570	A rare doubly nitrato and phenoxido bridged trimetallic Cu‹sup›II‹/sup› complex: EPR, antiferromagnetic coupling and theoretical rationalization. RSC Advances, 2016, 6, 54856-54865.	3.6	9
571	Introducing Supramolecular Interactions into Robust Bis(tetrabromocatecholate) Chelated Manganese(III) Systems and Biomimetic Catalytic Activity. ChemistrySelect, 2017, 2, 2094-2105.	1.5	9
572	A combined crystallographic and theoretical study of weak intermolecular interactions in crystalline squaric acid esters and amides. CrystEngComm, 2017, 19, 3071-3077.	2.6	9
573	The roles of H-bonding, Ï€-stacking, and antiparallel CO â‹¯ CO interactions in the formation of a new Gd(III) coordination polymer based on pyridine-2,6-dicarboxylic acid. Inorganic Chemistry Communication, 2017, 83, 24-26.	3.9	9
574	Theoretical investigation on molecular structure of a new mononuclear copper(II) thiocyanato complex with tridentate Schiff base ligand. Journal of Coordination Chemistry, 2017, 70, 3715-3726.	2.2	9
575	Influence of ancillary ligands on preferential geometry and biomimetic catalytic activity in manganese(III)-catecholate systems: A combined experimental and theoretical study. Journal of Inorganic Biochemistry, 2017, 176, 77-89.	3.5	9
576	Solvent dependent nuclearity of manganese complexes with a polydentate hydrazone-based ligand and thiocyanate anions. Inorganica Chimica Acta, 2017, 455, 204-212.	2.4	9

#	Article	IF	Citations
577	Bioactive Heterometallic Cu^{II}â€“Zn^{II} Complexes with Potential Biomedical Applications. ACS Omega, 2018, 3, 13343-13353.	3.5	9
578	Hydrogen bonding versus Ï€-interactions: their key competition in sildenafil solvates. CrystEngComm, 2018, 20, 4526-4530.	2.6	9
579	Crystal structures of N⁶-modified-aminoacid/peptide nucleobase analogs: hybrid adenineâ€“glycine and adenineâ€“glycylglycine molecules. New Journal of Chemistry, 2018, 42, 14742-14750.	2.8	9
580	Solid-state supramolecular architectures of a series of Hg(<scp>ii</scp>) halide coordination compounds based on hydroxyl-substituted Schiff base ligands. CrystEngComm, 2019, 21, 6301-6312.	2.6	9
581	Chloranilate bridged dinuclear copper(<scp>ii</scp>) complexes: synâ€“anti geometry tuned by the steric factor and supramolecular interactions. CrystEngComm, 2019, 21, 6886-6893.	2.6	9
582	Unravelling the electronic nature of Câ€“Fâ‹¯Oâ€“C non-covalent interaction in proteins and small molecules in the solid state. Physical Chemistry Chemical Physics, 2020, 22, 25704-25711.	2.8	9
583	Supramolecular architectures of Mn(NCS)2 complexes with N'-(1-(pyridin-4-yl)ethylidene)picolinohydrazide and N'-(phenyl(pyridin-4-yl)methylene)isonicotinohydrazide. Polyhedron, 2020, 190, 114776.	2.2	9
584	Novel Pb(II) Complexes: X-Ray Structures, Hirshfeld Surface Analysis and DFT Calculations. Crystals, 2020, 10, 568.	2.2	9
585	Ïƒ- and Ï€-Hole Interactions. Crystals, 2020, 10, 721.	2.2	9
586	Selective functionalisation of aromatic alcohols with supramolecularly regulated gold(<scp>i</scp>) catalysts. Organic Chemistry Frontiers, 2020, 7, 1626-1634.	4.5	9
587	Role of Imidazole Coâ€“Ligand in the Supramolecular Network of a Co(II) Complex with Sulfadiazine: Crystal Structure, Hirshfeld Surface Analysis and Energetic Calculations. ChemistrySelect, 2020, 5, 6331-6338.	1.5	9
588	Binuclear and tetranuclear Zn(<scp>ii</scp>) complexes with thiosemicarbazones: synthesis, X-ray crystal structures, ATP-sensing, DNA-binding, phosphatase activity and theoretical calculations. RSC Advances, 2020, 10, 12735-12746.	3.6	9
589	Synthesis, X-ray characterization, Hirshfeld surface analysis and DFT calculations on tetrazolyl-phenol derivatives: H-bonds vs Câ€“Hâ€¦Ï€/Ï€â€¦Ï€ interactions. Journal of Molecular Structure, 2021, 1227, 129425.	3.6	9
590	Existence of stronger C HÂ·Â·Â·Ï€(chelate ring) interaction compared to C HÂ·Â·Â·Ï€(arene) interactions in the supramolecular assembly of dinuclear iron(III) Schiff base complexes: A theoretical insight. Inorganica Chimica Acta, 2021, 516, 120081.	2.4	9
591	Supramolecular assemblies involving biologically relevant antiparallel Ï€-stacking and unconventional solvent driven structural topology in maleato and fumarato bridged Zn(<scp>ii</scp>) coordination polymers: antiproliferative evaluation and theoretical studies. New Journal of Chemistry, 2021, 45, 13040-13055.	2.8	9
592	Azine Steric Hindrances Switch Halogen Bonding to Nâ€Arylation upon Interplay with Ïƒâ€Hole Donating Haloarenenitriles. Chemistry - an Asian Journal, 2021, 16, 1445-1455.	3.3	9
593	Molecular Electrostatic Potential and Noncovalent Interactions in Derivatives of Group 8 Elements. Angewandte Chemie, 2021, 133, 20891-20895.	2.0	9
594	Bifunctional Fluorophosphonium Triflates as Intramolecular Frustrated Lewis Pairs: Reversible CO₂ Sequestration and Binding of Carbonyls, Nitriles and Acetylenes. Chemistry - A European Journal, 2021, 27, 13709-13714.	3.3	9

#	Article	IF	Citations
595	Benzoato bridged dinuclear Mn(II) and Cu(II) compounds involving guest chlorobenzoates and dimeric paddle wheel supramolecular assemblies: Antiproliferative evaluation and theoretical studies. Polyhedron, 2021, 208, 115409.	2.2	9
596	Enhancing chalcogen bonding by metal coordination. Dalton Transactions, 2022, , .	3.3	9
597	Do 2-coordinate iodine(<scp>i</scp>) and silver(<scp>i</scp>) complexes form nucleophilic iodonium interactions (NIIs) in solution?. Chemical Communications, 2022, 58, 4977-4980.	4.1	9
598	Novel Polymorphic Cocrystals of the Non-Steroidal Anti-Inflammatory Drug Niflumic Acid: Expanding the Pharmaceutical Landscape. Pharmaceutics, 2021, 13, 2140.	4.5	9
599	Inorganicâ€“organic {d_{z²}-M^{II}S₄}â‹Ï€-hole stacking in reverse sandwich structures: the case of cocrystals of group 10 metal dithiocarbamates with electron-deficient arenes. Inorganic Chemistry Frontiers, 2022, 9, 2869-2879.	6.0	9
600	The generation of C,O,O-trilithiated derivatives of dihydric phenols. Tetrahedron Letters, 1991, 32, 7313-7316.	1.4	8
601	Self-assembly of [2]Rotaxane Exploiting Reversible Pt(II)- Pyridine Coordinate Bonds. Molecules, 2004, 9, 278-286.	3.8	8
602	Applicability of the 1H NMR chemical shifts computed by the ab initio/GIAO-HF methodology to the study of geometrical features of Zn-porphyrin dimers. Tetrahedron Letters, 2004, 45, 9387-9391.	1.4	8
603	Synthesis, X-ray characterization and computational studies of Cu(ii) complexes of N-pyrazolyl pyrimidine. Dalton Transactions, 2012, 41, 11161.	3.3	8
604	Synthesis, X-ray characterization and computational Studies of N-imidazolyl and N-pyrazolyl pyrimidine derivatives. Tetrahedron, 2012, 68, 2374-2382.	1.9	8
605	Experimental and theoretical study of N1-hexylcytosine and N1-hexylcytosinium nitrate: the crucial role of hydrophobic and anionâ€“Ï€ interactions. Tetrahedron Letters, 2013, 54, 5355-5360.	1.4	8
606	Anion-Ï€ Interactions in Supramolecular Chemistry and Catalysis. Challenges and Advances in Computational Chemistry and Physics, 2015, , 471-500.	0.6	8
607	Synthesis, crystal structures, magnetic properties and DFT calculations of nitrate and oxalate complexes with 3,5 dimethyl-1-(2â€²-pyridyl)-pyrazole-Cu(<scp>ii</scp>). RSC Advances, 2015, 5, 45082-45091.	3.6	8
608	Solvent-controlled construction of manganese(II) complexes with 4-acetylpyridine nicotinoylhydrazone ligand. Inorganica Chimica Acta, 2015, 438, 220-231.	2.4	8
609	The first mixed-ligand coordination compound involving 8-aminoquinoline and pyridine-2,6-dicarboxylate: synthesis, X-ray crystal structure, and DFT studies. Journal of Coordination Chemistry, 2015, 68, 3599-3610.	2.2	8
610	Anion-dependent structural diversity of cadmium(II) complexes: synthesis, crystal structures, luminescence properties, and unusual C-H/Ï*f* supramolecular interactions involving Ï*f*-aromatic M₂X₂ cores. Journal of Coordination Chemistry, 2016, 69, 1188-1205.	2.2	8
611	Coordination Behavior of Chelidamic Acid With V^V, Ni^{II}, Fe^{III}, and Ca^{II}: Syntheses, Xâ€ray Characterization and DFT Studies. ChemistrySelect, 2016, 1, 1556-1566.	1.5	8
612	Weak interactions within nitryl halide heterodimers. New Journal of Chemistry, 2016, 40, 9060-9072.	2.8	8

#	Article	IF	Citations
613	Copper(II) pseudohalide complexes with isomeric N₂O donor Schiff base ligands: Synthesis, characterization and molecular dynamics simulations of interactions with DNA. ChemistrySelect, 2016, 1, 448-455.	1.5	8
614	Donorâ€“acceptor interactions in tri(phosphonio)methanide dications [(Ph3P)2CP(X)Ph2]2+(X = H, Me,) Tj ETQq0 0 0 rgBT /Overlock 1	3.3	8
615	Experimental and computational investigations of the photosensitive Schottky barrier diode property of an azobenzene based small organic molecule. New Journal of Chemistry, 2018, 42, 13430-13441.	2.8	8
616	Synthesis of Multinuclear Zn(II) Complexes Involving 8â€Aminoquinolineâ€•Based Schiffâ€Base Ligand: Structural Diversity, DNA Binding Studies and Theoretical Calculations.. ChemistrySelect, 2018, 3, 7697-7706.	1.5	8
617	A family of [Cu2], [Cu4] and [Cu5] aggregates: alteration of reaction conditions, ancillary bridges and capping anions. New Journal of Chemistry, 2018, 42, 14349-14364.	2.8	8
618	Tri-nuclear copper-cadmium complexes of a N2O2-donor ligand with the variation of counter anions: Structural elucidation and theoretical study on inter-molecular interactions. Inorganica Chimica Acta, 2019, 492, 142-149.	2.4	8
619	On the Role of Water as a Catalyst in Prebiotic Chemistry. ChemPhysChem, 2020, 21, 313-320.	2.1	8
620	9-Ethyladenine: Mechanochemical Synthesis, Characterization, and DFT Calculations of Novel Cocrystals and Salts. Crystal Growth and Design, 2020, 20, 2985-2997.	3.0	8
621	Semiconducting properties of pyridyl appended linear dicarboxylate based coordination polymers: theoretical prediction via DFT study. Dalton Transactions, 2021, 50, 270-278.	3.3	8
622	A supramolecular 3D structure constructed from a new metal chelate self-assembled from Sn(NCS)2 and phenyl(pyridin-2-yl)methylenepicolinohydrazide. Journal of Molecular Structure, 2021, 1224, 129188.	3.6	8
623	Unprecedented [d9]Cuâ‹¯[d10]Au coinage bonding interactions in {Cu(NH3)4[Au(CN)2]}+[Au(CN)2]â^' salt. Chemical Communications, 2021, 57, 7268-7271.	4.1	8
624	Insight into non-covalent interactions in two triamine-based mononuclear iron(<scp>iii</scp>) Schiff base complexes with special emphasis on the formation of Brâ‹¯Ï€ halogen bonding. CrystEngComm, 2021, 23, 1578-1587.	2.6	8
625	An experimental and theoretical exploration of supramolecular interactions and photoresponse properties of two Ni(<scp>ii</scp>) complexes. New Journal of Chemistry, 2021, 45, 12108-12119.	2.8	8
626	On the importance of RH₃Câ‹¯N tetrel bonding interactions in the solid state of a dinuclear zinc complex with a tetradentate Schiff base ligand. CrystEngComm, 2021, 23, 3391-3397.	2.6	8
627	Weak Interactions in Cocrystals of Isoniazid with Glycolic and Mandelic Acids. Crystals, 2021, 11, 328.	2.2	8
628	An insight to the spin density distribution and non-covalent interactions in a carboxylate bridged class-I mixed valence cobalt(II),cobalt(III) complex of quadruplet nature. Inorganica Chimica Acta, 2021, 521, 120298.	2.4	8
629	Unconventional enclathration of guest adipic acid and energetically significant antiparallel Ï€-stacked ternary assemblies involving unusual regium-Ï€(chelate) contacts in phenanthroline-based Ni(II) and Cu(II) compoundsâ€"Antiproliferative evaluation and theoretical studies. Journal of Molecular Structure, 2021, 1245, 131038.	3.6	8
630	Phenoxido mediated antiferromagnetic and azide mediated ferromagnetic coupling in two dinuclear ferromagnetic nickel(<scp>ii</scp>) complexes with isomeric Schiff bases: a theoretical insight on the pathway of magnetic interaction. CrystEngComm, 2021, 23, 1942-1952.	2.6	8

#	Article	IF	Citations
631	Spodium bonds and metalâ€“halogenÂ·Â·Â·halogenâ€“metal interactions in propagation of monomeric units to dimeric or polymeric architectures. Journal of Molecular Structure, 2022, 1252, 132144.	3.6	8
632	Expanding the toolbox of the coinage bond: adducts involving new gold(<scp>iii</scp>) derivatives and bioactive molecules. CrystEngComm, 2022, 24, 3846-3851.	2.6	8
633	Intramolecular noncovalent force in cyclic amidines: nonbonded interaction between carbon atoms and heteroatoms. Chemical Physics Letters, 2003, 372, 489-496.	2.6	7
634	Theoretical ab initio study of substituted benzene trimer: Interplay between hydrogen bonding and Ï€â€“Ï€ interactions. Computational and Theoretical Chemistry, 2011, 975, 106-110.	2.5	7
635	Theoretical ab initio study of lone pair and anionâ€“Ï€ interactions in fluorinated tropolones. Computational and Theoretical Chemistry, 2012, 998, 20-25.	2.5	7
636	On the relationship between ring strain energies and â€˜atoms-in-moleculesâ€™ properties in N2P2 rings. Chemical Physics Letters, 2014, 597, 40-44.	2.6	7
637	An unusual nitrosoâ‹¯nitroso interaction in the coordination polymer structures of Ni(<scp>ii</scp>) and Co(<scp>ii</scp>) complexes with the Î±,Ï‰-bis(benzotriazoloxy)alkane system. CrystEngComm, 2014, 16, 654-666.	2.6	7
638	Synthetic Modulation of a Chemosensor Affords Target Metal Ion Switch from Zn2+to Al3+. ChemistrySelect, 2017, 2, 5414-5420.	1.5	7
639	Copper(II) polyamine chelates as efficient receptors for acyclovir: syntheses, crystal structures and dft study. Polyhedron, 2018, 145, 218-226.	2.2	7
640	Throughâ€Space â€œÎ±â€Effectâ€•between the Bridging Oxygen Atoms in Diepoxybenzo[de]isothiochromene Derivatives. European Journal of Organic Chemistry, 2020, 2020, 156-161.	2.4	7
641	Influence of 2-Amino-4-methylpyridine and 2-Aminopyrimidine Ligands on the Malonic Acid-Cu(II) System: Insights through Supramolecular Interactions and Photoresponse Properties. ACS Omega, 2020, 5, 460-470.	3.5	7
642	Metalâ€“organic architectures driven by a multifunctional 6-aminouracil spacer: structures, noncovalent interactions, and conductivity. CrystEngComm, 2020, 22, 829-840.	2.6	7
643	Recurrent Ï€(arene)â‹¯Ï€(chelate ring) motifs in four trinuclear CuII2MII (M = Cd/Zn) complexes derived from an unsymmetrical N2O2 donor ligand: structural and theoretical investigations. CrystEngComm, 2020, 22, 7673-7683.	2.6	7
644	In-vitro prediction of the membranotropic action of emerging organic contaminants using a liposome-based multidisciplinary approach. Science of the Total Environment, 2020, 738, 140096.	8.0	7
645	Synthesis, X-ray characterization and theoretical study of 3a,6:7,9a-diepoxybenzo[de]isoquinoline derivatives: on the importance of Fâ‹¯O interactions. New Journal of Chemistry, 2020, 44, 20167-20180.	2.8	7
646	Two copper (II) complexes derived from anthranilic acid and 4-iodo-anthranilic acid Schiff bases: Structural elucidation, halogen bonding interactions and catalytic study using 3,5-DTBC. Journal of Molecular Structure, 2020, 1217, 128398.	3.6	7
647	Iridium(III) coordination of N(6) modified adenine derivatives with aminoacid chains. Journal of Inorganic Biochemistry, 2020, 205, 111000.	3.5	7
648	New metal chelate constructed from Ni(NCS)2 and 1,2-diphenyl-1,2-bis((phenyl(pyridin-2-yl)methylene)hydrazono)ethane. Inorganica Chimica Acta, 2020, 509, 119707.	2.4	7

#	Article	IF	Citations
649	Straightforward Three-Component Synthesis of Nâ€²,Nâ€²â€²-Disubstituted N-Alkyl-1,3,5-Triazinanes. Synlett, 2020, 31, 1067-1072.	1.8	7
650	An insight into the role of supramolecular interactions to stabilize the solid state structure of an octahedral nickel(II) diamine complex. Inorganica Chimica Acta, 2021, 515, 120023.	2.4	7
651	A convenient access to fluorophosphonium triflate salts by electrophilic fluorination and anion exchange. Inorganic Chemistry Frontiers, 2021, 8, 2854-2864.	6.0	7
652	Short XÂ·Â·Â·N Halogen Bonds With Hexamethylenetetraamine as the Acceptor. Frontiers in Chemistry, 2021, 9, 623595.	3.6	7
653	Using Room Temperature Phosphorescence of Gold(I) Complexes for PAHs Sensing. Molecules, 2021, 26, 2444.	3.8	7
654	Uracil Derivatives for Halogen-Bonded Cocrystals. International Journal of Molecular Sciences, 2021, 22, 10663.	4.1	7
655	Understanding the planar conformations in diarylsubstituted heteroarenes: structural and theoretical insights. CrystEngComm, 2021, 23, 3144-3151.	2.6	7
656	Lead(<scp>ii</scp>) supramolecular structures formed through a cooperative influence of the hydrazinecarbothioamide derived and ancillary ligands. CrystEngComm, 2022, 24, 368-378.	2.6	7
657	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
658	An insight into triel bonds in O,Oâ€²-diarylphosphorodithioates of thallium(<scp>i</scp>): experimental and theoretical investigations. New Journal of Chemistry, 2022, 46, 832-843.	2.8	7
659	Structural topologies involving energetically significant antiparallel Ï€-stacking and unconventional N(nitrile)â‹¯Ï€(fumarate) contacts in dinuclear Zn(<scp>ii</scp>) and polymeric Mn(<scp>ii</scp>) compounds: antiproliferative evaluation and theoretical studies. New Journal of Chemistry, 2022, 46, 5296-5311.	2.8	7
660	Insight into non-covalent interactions in a [Cu(N₃)₄]^{2â^'} bridged hetero-pentanuclear copper(<scp>ii</scp>)/sodium complex with special emphasis on the strong CHâ‹¯Ï€[Cu(N₃)₄] interactions. New Journal of Chemistry, 2022, 46, 11286-11295.	2.8	7
661	Predicting experimental complexation-induced changes in NMR chemical shift for complexes between metalloporphyrins and ligands using the Ab initio/GIAO-HF methodology. Chemical Physics Letters, 2002, 360, 72-78.	2.6	6
662	Analyses of supramolecular interactions present in a coordination polymer of Mn(II) with 2-picolinate and 4,4â€²-Azobis(pyridine). Inorganic Chemistry Communication, 2014, 41, 1-5.	3.9	6
663	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. Dalton Transactions, 2014, 43, 6353.	3.3	6
664	A new oxo centered basic p-chlorobenzoate bridging heterotrinuclear complex, [Cr2MnO(C7H4O2Cl)6(Py)3]C7H5O2Cl: Synthesis, X-ray crystal structure and theoretical DFT study. Polyhedron, 2014, 81, 349-355.	2.2	6
665	A new solvated complex of the uranyl ion (UO22+) with 8-hydroxyquinoline. Inorganica Chimica Acta, 2015, 426, 136-141.	2.4	6
666	A trigonal prismatic anionic iron(<scp>iii</scp>) complex of a radical o-iminobenzosemiquinonate derivative: structural and spectral analyses. New Journal of Chemistry, 2017, 41, 7283-7291.	2.8	6

#	Article	IF	Citations
667	Synthesis, structures, and investigation of noncovalent interactions of 1,3-dimethyl-5-(4Ê¹/3Ê¹-pyridylazo)-6-aminouracil and their Ni(II) complexes. Journal of Molecular Structure, 2018, 1170, 70-81.	3.6	6
668	Synthesis, structural features, antibacterial behaviour and theoretical investigation of two new manganese(III) Schiff base complexes. Polyhedron, 2018, 151, 407-416.	2.2	6
669	Spectral, electrochemical and DFT studies of a trimetallic CuII Derivative: Antimycobacterial and cytotoxic activity. Inorganica Chimica Acta, 2019, 490, 155-162.	2.4	6
670	EPR, DFT and electrochemical interpretation of a Cu(II) derivative incorporating a Schiff base precursor. Polyhedron, 2019, 159, 323-329.	2.2	6
671	Synthesis, reactivity, X-ray characterization and docking studies of N7/N9-(2-pyrimidyl)-adenine derivatives. Journal of Inorganic Biochemistry, 2020, 203, 110879.	3.5	6
672	Insight into the formation of H-bonds propagating the monomeric zinc complexes of a tridentate reduced Schiff base to form an infinite chain. CrystEngComm, 2021, 23, 1918-1928.	2.6	6
673	Charge Assisted Hydrogen Bonded Assemblies and Unconventional Oâˆ™âˆ™âˆ™O Dichalcogen Bonding Interactions in Pyrazole-Based Isostructural Ni(II) and Mn(II) Compounds involving Anthraquinone Disulfonate: Antiproliferative Evaluation and Theoretical Studies. Journal of Molecular Structure, 2021, 1250, 131883.	3.6	6
674	Synthesis, structural topologies and anticancer evaluation of phenanthroline-based 2,6-pyridinedicarboxylato Cu(II) and Ni(II) compounds. Polyhedron, 2022, 213, 115632.	2.2	6
675	Hostâ€“guest complexesvs.supramolecular polymers in chalcogen bonding receptors: an experimental and theoretical study. Dalton Transactions, 2022, 51, 1325-1332.	3.3	6
676	Iodine(<scp>i</scp>) complexes incorporating sterically bulky 2-substituted pyridines. RSC Advances, 2022, 12, 8674-8682.	3.6	6
677	Substituent Effects in Ï€â€Hole Regium Bonding Interactions Between Au(p â€Xâ€Py) ₂ Complexes and Lewis Bases: An ab initio Study. ChemPhysChem, 2022, , .	2.1	6
678	Investigation of solid state architectures in tetrazolyl tryptophol stabilized by crucial aromatic interactions and hydrogen bonding: Experimental and theoretical analysis. Journal of Molecular Structure, 2022, 1262, 133079.	3.6	6
679	Role of Redox-Inactive Metal Ions in Modulating the Reduction Potential of Uranyl Schiff Base Complexes: Detailed Experimental and Theoretical Studies. Inorganic Chemistry, 2022, 61, 7130-7142.	4.0	6
680	Quadrupole moment versus Molecular Electrostatic Potential: Strange behavior of ethynyl-substituted benzenes. Chemical Physics Letters, 2013, 567, 60-65.	2.6	5
681	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. Journal of Molecular Structure, 2015, 1079, 78-86.	3.6	5
682	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. Polyhedron, 2017, 134, 153-165.	2.2	5
683	Mononuclear and dinuclear trimethylplatinum(<scp>iv</scp>) iodide complexes of 3-substituted pyridines. New Journal of Chemistry, 2017, 41, 3498-3507.	2.8	5
684	Zinc(ii) complexes with uncommon aminal and hemiaminal ether derivatives: synthesis, structure, phosphatase activity and theoretical rationalization of ligand and complex formation. New Journal of Chemistry, 2018, 42, 12998-13009.	2.8	5

#	Article	IF	Citations
685	Synchronized On/Off Switching of Four Binding Sites for Water in a Molecular Solomon Link. Angewandte Chemie, 2019, 131, 8137-8141.	2.0	5
686	Halogen interactions in dinuclear copper(II) 2,4-dibromophenoxyacetate â€“ crystal structure and quantum chemical calculations. Journal of Molecular Structure, 2020, 1202, 127227.	3.6	5
687	Molecular and supramolecular recognition patterns in ternary copper(II) or zinc(II) complexes with selected rigid-planar chelators and a synthetic adenine-nucleoside. Journal of Inorganic Biochemistry, 2020, 203, 110920.	3.5	5
688	Naphthalenediimides with Cyclic Oligochalcogenides in Their Core. Chemistry - A European Journal, 2020, 26, 14059-14063.	3.3	5
689	Raise the anchor! Synthesis, X-ray and NMR characterization of 1,3,5-triazinanes with an axial tert-butyl group. Organic and Biomolecular Chemistry, 2020, 18, 8386-8394.	2.8	5
690	Crystal structures of N⁶-modified-amino acid nucleobase analogs(<scp>iii</scp>): adenineâ€“valeric acid, adenineâ€“hexanoic acid and adenineâ€“gabapentine. New Journal of Chemistry, 2020, 44, 12236-12246.	2.8	5
691	Complexes of BiCl₃ with hydrazone derived ligands: a MÃ¶bius-like discrete metal chelate versus a salt-like porous polymeric structure. New Journal of Chemistry, 2020, 44, 9429-9437.	2.8	5
692	Selective Metalâ€“Ligand Bond-Breaking Driven by Weak Intermolecular Interactions: From Metamagnetic Mn(III)-Monomer to Hexacyanoferrate(II)-Bridged Metamagnetic Mn₂Fe Trimer. Inorganic Chemistry, 2020, 59, 8487-8497.	4.0	5
693	A combined experimental and theoretical study on an ionic cobalt(III/II) complex with a Schiff base ligand. Polyhedron, 2020, 182, 114432.	2.2	5
694	Anion-dependent structural variations and charge transport property analysis of 4â€²-(3-pyridyl)-4,2â€²:6â€²,4â€²â€²-terpyridinium salts. CrystEngComm, 2021, 23, 3569-3581.	2.6	5
695	Ligand Steric Hindrances Switch Bridging (Î¼₂-I)Â·Â·Â·O,O to Two-Center IÂ·Â·Â·O Halogen-Bonding Mode in the Assembly of Diketonate Copper(II) Species. Crystal Growth and Design, 2021, 21, 4073-4082.	3.0	5
696	Importance of Anionâˆ’Ï€ Interactions in RNA GAAA and GGAG Tetraloops: A Combined MD and QM Study. Journal of Chemical Theory and Computation, 2021, 17, 6624-6633.	5.3	5
697	Metalloid Chalcogenâ€“pnictogen Ïƒ-hole bonding competition in stibanyl telluranes. Journal of Organometallic Chemistry, 2021, 954-955, 122092.	1.8	5
698	Frontispiece: Metal Centers as Nucleophiles: Oxymoron of Halogen Bondâ€Involving Crystal Engineering. Chemistry - A European Journal, 2022, 28, .	3.3	5
699	Aza-Crown-Based Macrocyclic Probe Design for â€œPET-offâ€•Multi-Cu²⁺ Responsive and â€œCHEF-onâ€•Multi-Zn²⁺ Sensor: Application in Biological Cell Imaging and Theoretical Studies. Inorganic Chemistry, 2022, 61, 1982-1996.	4.0	5
700	Field-induced single-molecule magnet behaviour in a series of dinuclear cobalt(III,II) complexes. Polyhedron, 2022, 220, 115802.	2.2	5
701	Exploration of noncovalent interactions in the solid state structures of carboxylate bridged trinuclear mixed valence cobalt complexes using computational tools based on the topological analysis of the electron density. Polyhedron, 2022, 223, 115910.	2.2	5
702	Exploration of supramolecular and theoretical aspects of two new Cu(II) complexes: On the importance of lone pairÂ·Â·Â·Ï€(chelate ring) and Ï€Â·Â·Â·Ï€(chelate ring) interactions. Journal of Molecular Structure, 2022, 1265, 133358.	3.6	5

#	Article	IF	Citations
703	Centroidâ‹¯centroid and hydrogen bond interactions as robust supramolecular units for crystal engineering: X-ray crystallographic, computational and urease inhibitory investigations of 1,2,4-triazolo[3,4-a]phthalazines. CrystEngComm, 0, , .	2.6	5
704	Synthesis, characterization and self assembly of dinuclear zinc Schiff base complexes: A combined experimental and theoretical study. Polyhedron, 2022, 225, 116044.	2.2	5
705	Affinity of ferrocene and (1,1â€²)(3,3â€²)[3,3]ferrocenophane to cations. Chemical Physics Letters, 2006, 424, 204-208.	2.6	4
706	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
707	Copperâ€Assisted Hemiacetal Synthesis: A Cu^{II} Chain Obtained by a Oneâ€Step in situ Reaction of Picolinaldehyde. European Journal of Inorganic Chemistry, 2014, 2014, 3271-3278.	2.0	4
708	An experimental and computational investigations of supramolecular anionâ€“Ï€/Ï€â€“Ï€/Ï€â€“anion assemblies in mononuclear Zn(II) complexes with a versatile tetradentate N-donor Schiff base ligand. Polyhedron, 2015, 102, 764-772.	2.2	4
709	A Ni(II) derivative incorporating tetradentate Schiff base precursor: Structure, spectral, electrochemical and DFT interpretation. Journal of Molecular Structure, 2018, 1173, 462-468.	3.6	4
710	Exploiting 1,4-naphthoquinone and 3-iodo-1,4-naphthoquinone motifs as anion binding sites by hydrogen or halogen-bonding interactions. Dalton Transactions, 2019, 48, 11813-11821.	3.3	4
711	Zn(II) and Co(II) derivatives anchored with scorpionate precursor: Antiproliferative evaluation in human cancer cell lines. Journal of Inorganic Biochemistry, 2020, 202, 110881.	3.5	4
712	Combined experimental and computational studies on preferential CO₂ adsorption over a zinc-based porous framework solid. New Journal of Chemistry, 2020, 44, 1806-1816.	2.8	4
713	Intramolecular sp2-sp3 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. Crystals, 2020, 10, 369.	2.2	4
714	Anionâ€“Cation Recognition Pattern, Thermal Stability and DFT-Calculations in the Crystal Structure of H2dap[Cd(HEDTA)(H2O)] Salt (H2dap = H2(N3,N7)-2,6-Diaminopurinium Cation). Crystals, 2020, 10, 304.	2.2	4
715	Ligand structure-driven self-assembly of Zn(NCS)2 with a carbohydrazone ligand: A possible intermediate towards a [2ÂÃ—Â2] metallic grid. Journal of Molecular Structure, 2021, 1225, 129269.	3.6	4
716	Ultrashort HÎ´+â‹¯HÎ´â¯ intermolecular distance in a supramolecular system in the solid state. Chemical Communications, 2021, 57, 7112-7115.	4.1	4
717	H-Bonds, Ï€-Stacking and (Water)O-H/Ï€ Interactions in (Âµ4-EDTA)Bis(Imidazole) Dicopper(II) Dihydrate. Crystals, 2021, 11, 48.	2.2	4
718	Anionâ‹…â‹…â‹…Anion Coinage Bonds: The Case of Tetrachloridoaurate. Angewandte Chemie, 2021, 133, 14506-14510.	2.0	4
719	Molecular 1,1â€²-bifunctional mixed-valence Pâ€“P compounds, enabled through metal complexation. Dalton Transactions, 2021, 50, 2131-2137.	3.3	4
720	A combined theoretical and CSD perspective on Ï*f*-hole interactions with tetrels, pnictogens, chalcogens, halogens, and noble gases. , 2021, , 119-155.		4

#	Article	IF	Citations
721	On the nature of recurrent Auâ‹¯Ï€ motifs in tris(2,2â€²-bipyridine)M(<scp>ii</scp>) (M = Fe, Co and Ni) dicyanoaurate(<scp>i</scp>) salts: X-ray analysis and theoretical rationalization. Dalton Transactions, 2021, 50, 16954-16960.	3.3	4
722	CHAPTER 9. Quantitative Analysis of Weak Non-covalent Ïƒ-Hole and Ï€-Hole Interactions. Monographs in Supramolecular Chemistry, 2018, , 285-333.	0.2	4
723	Multicomponent Solids of DL-2-Hydroxy-2-phenylacetic Acid and Pyridinecarboxamides. Crystals, 2022, 12, 142.	2.2	4
724	Solvent-driven structural topologies in phenanthroline-based co-crystals of Zn(<scp>ii</scp>) involving fascinating infinite chair-like {[(bzH)₄Cl₂]^{2â^'}}_nassemblies and unconventional layered infinite {bz-H₂O-Cl}_nanion-water clusters: antiproliferative evaluation and theoretical studies. New Journal of Chemistry, 2022, 46, 5638-5652.	2.8	4
725	Supramolecular aggregation of lead(II) perchlorate and a thiosemicarbazide derivative linked by a myriad of non-covalent interactions. Inorganica Chimica Acta, 2022, 538, 120974.	2.4	4
726	Estimation of the ability of the Ï€-system of pseudohalides (azide and thiocyanate) to participate in CHÂ·Â·Â·Ï€ interactions in cyclic hetero-tetranuclear cobalt(III)/sodium and linear trinuclear mixed valence cobalt(III/II/III) complexes. Polyhedron, 2022, 222, 115862.	2.2	4
727	Antiparallel Ï€Â·Â·Â·Ï€ and Câ^'HÂ·Â·Â·Hâ^'C contacts in a novel Zn(II) coordination solid involving Ï€-hole tetrel bonding interactions: A combined experimental and theoretical study, Hirshfeld surface analysis, molecular docking and potential drug property. Journal of Molecular Structure, 2022, 1268, 133686.	3.6	4
728	The Role of the Ethynyl Substituent on the Ï€â€“Ï€ Stacking Affinity of Benzene: A Theoretical Study. ChemPhysChem, 2011, 12, 283-288.	2.1	3
729	Electronic Structure of N₂P₂ Fourâ€Membered Rings. ChemPhysChem, 2014, 15, 1599-1603.	2.1	3
730	Pseudohalides regulated diverse helicity in copper(II) coordination polymers derived from a bis(aminoethoxy) ligand. Polyhedron, 2017, 124, 262-274.	2.2	3
731	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. Inorganica Chimica Acta, 2017, 461, 183-191.	2.4	3
732	Ambiguous reactivity of Li/Cl phosphinidenoid complexes under redox conditions â€“ a novel dichotomy in phosphorus chemistry. Chemical Communications, 2017, 53, 933-936.	4.1	3
733	Ni-Catalysed Intramolecular [4+4]-cycloadditions of bis-dienes towards eight-membered fused bicyclic systems: a combined experimental and computational study. Catalysis Science and Technology, 2018, 8, 5251-5258.	4.1	3
734	Surface Modification of Pseudoboehmite-Coated Aluminum Plates with Squaramic Acid Amphiphiles. ACS Omega, 2019, 4, 14868-14874.	3.5	3
735	Synthesis and characterization of a manganese(III) schiff base complex and exploration of BrÂ·Â·Â·Br interaction in the solid state structure of the complex. Journal of Coordination Chemistry, 2019, 72, 3237-3247.	2.2	3
736	Synthesis, structural and DFT interpretation of a Schiff base assisted Mn(III) derivative. Journal of Molecular Structure, 2020, 1199, 126985.	3.6	3
737	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. Molecules, 2020, 25, 285.	3.8	3
738	DFT analysis of supra-molecular assemblies of substituted 4H-pyran derivatives. Journal of Molecular Structure, 2020, 1207, 127785.	3.6	3

#	Article	IF	Citations
739	Toward N,P-Doped Ï€-Extended PAHs: A One-Pot Synthesis to Diannulated 1,4,2-Diazaphospholium Triflate Salts. Journal of Organic Chemistry, 2020, 85, 14420-14434.	3.2	3
740	A first exploration of isostructurality in transition metal nitroprussides: X-ray analysis, magnetic properties and DFT calculations. CrystEngComm, 2021, 23, 1158-1171.	2.6	3
741	Dicopper(II)-EDTA Chelate as a Bicephalic Receptor Model for a Synthetic Adenine Nucleoside. Pharmaceuticals, 2021, 14, 426.	3.8	3
742	Frustrated Lewis Pairs based on CarbonÂ·Â·Â·Carbon+ tetrel bonds: A DFT study. MarÃa de las Nieves PiÃ±a[a], Antonio Frontera[a], Tiddo. J. Mooibroek[b],* and Antonio BauzÃ¡*[a]. ChemPhysChem, 2021, 22, 2478-2483.	2.1	3
743	Change in molecular shapes of the trinuclear CuII2ZnII complexes on Schiff base reduction: structural and theoretical investigations. CrystEngComm, 2021, 23, 4848-4856.	2.6	3
744	Energetic features of antiparallel stacking and hydrogen bonding interactions in two coordination complexes bearing 1,10-phenanthroline-2,9-dicarboxylic acid. Journal of Molecular Structure, 2022, 1251, 131963.	3.6	3
745	Oxalic Acid, a Versatile Coformer for Multicomponent Forms with 9-Ethyladenine. Crystals, 2022, 12, 89.	2.2	3
746	Static discrete disorder in the crystal structure of iododiflunisal: on the importance of hydrogen bond, halogen bond and Ï€-stacking interactions. CrystEngComm, 0, , .	2.6	3
747	On metal coordination of neutral open-shell P-ligands focusing on phosphanoxyls, their electron residence and reactivity. Chemical Communications, 2022, 58, 6270-6279.	4.1	3
748	Terephthalato and succinato bridged Mn(II) and Zn(II) coordination polymers involving structure-guiding H-bonded tetrameric assemblies: Antiproliferative evaluation and theoretical studies. Polyhedron, 2022, 224, 115982.	2.2	3
749	Internal rotation in squaramide and related compounds. A theoretical ab initio study. Theoretical Chemistry Accounts, 2002, 108, 157-167.	1.4	2
750	Kinetics and mechanism of the oxidation of hydroxylamine by a {Mn3O4}4+ core in aqueous acidic media. Dalton Transactions, 2011, 40, 9571.	3.3	2
751	A Highly Selective Fluorescence Turn-on Probe for Zn2+ Based on New Diaryloxadiazole Chelate. Chemistry Letters, 2011, 40, 1163-1164.	1.3	2
752	A new benzimidazolium incorporated chemodosimeter affording dual chromogenic and fluorescence switch-on signaling for the selective targeting of cyanide. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2013, 76, 293-300.	1.6	2
753	New chloride-dimethylsulfoxide-iridium(III) complex with histaminium. Polyhedron, 2015, 102, 735-740.	2.2	2
754	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
755	Selective and Reversible Fluoride Complexation from Water by a Cyclic Tri(phosphonio)methanide Dication. Angewandte Chemie, 2017, 129, 8015-8019.	2.0	2
756	Isolation of Azadiphosphiridines and Diphosphenimines by Cycloaddition of Azides and a Cationic Diphosphene. Angewandte Chemie, 2017, 129, 6314-6318.	2.0	2

#	Article	IF	Citations
757	Cu(II)â€“N6-Alkyladenine Complexes: Synthesis, X-ray Characterization and Magnetic Properties. Magnetochemistry, 2018, 4, 24.	2.4	2
758	A New phenoxido/trifluoroacetato bridged heterometallic NiII2CuII derivative: Structure, EPR interpretation and DFT computation. Journal of Molecular Structure, 2019, 1175, 948-955.	3.6	2
759	From Pâ€Functional Thiazolâ€2â€thione Derivatives to Phosphaalkenes. European Journal of Inorganic Chemistry, 2019, 2019, 1697-1705.	2.0	2
760	Metal removal from the secondary building unit of bio-MOF-1 by adenine N6-alkylation while retaining the overall 3D porous topology. CrystEngComm, 2020, 22, 4201-4205.	2.6	2
761	Novel Cd (II) Coordination Polymers Afforded with EDTA or Trans-1,2-Cdta Chelators and Imidazole, Adenine, or 9-(2-Hydroxyethyl) Adenine Coligands. Crystals, 2020, 10, 391.	2.2	2
762	Dual role of silver in a fluorogenic N-squaraine probe based on Ag(<scp>i</scp>)â€“Ï€ interactions. Dalton Transactions, 2021, 50, 9367-9371.	3.3	2
763	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 Î±-effect. CrystEngComm, 0, , .	2.6	2
764	Catecholase-Like Activity and Theoretical Study in Solid State of a New Ru(III)-Schiff Base Complex. Acta Chimica Slovenica, 2021, 68, 212-221.	0.6	2
765	1-Ethyluracil, a New Scaffold for Preparing Multicomponent Forms: Synthesis, Characterization, and Computational Studies. Crystal Growth and Design, 2021, 21, 4857-4870.	3.0	2
766	Solvent driven structural topologies involving unconventional O H(methanol)â‹¯Ï€ contact and anti-cooperative HBâ‹¯anion-Ï€â‹¯HB assemblies with unusual enclathration of dual guest (H2O)4 cores in Mn(II) and Ni(II) coordination compounds: Antiproliferative evaluation and theoretical studies. Polyhedron, 2021, 210, 115503.	2.2	2
767	An insight into the supramolecular interactions in two linear polyvanadates. Journal of Molecular Structure, 2021, 1242, 130681.	3.6	2
768	OPLS all-atom force field for carbohydrates. , 1997, 18, 1955.		2
769	Molecular Recognition of Carbohydrates: Interaction of Diols with Acetate Ion. , 1996, , 115-126.		2
770	A homonuclear Ï€-system with a singlet carbene-type Î± and a nucleophilic Î² phosphorus â€“ the first use in P-heterocyclic synthesis. Dalton Transactions, 2021, 50, 17892-17896.	3.3	2
771	Large interaction energy for the homodimer and the heterodimer extracted from the supramolecular chain of a bent trinuclear zinc(<scp>ii</scp>) complex with a reduced Schiff base ligand. New Journal of Chemistry, 2022, 46, 1845-1856.	2.8	2
772	Anion-Ï€ stacks of Lindqvist superoctahedra [Mo6O19]2â^' supported by caffeinium and theophyllinium cations. Inorganica Chimica Acta, 2022, 537, 120945.	2.4	2
773	Osme bond: anisotropic distribution of electron density in action. Acta Crystallographica Section A: Foundations and Advances, 2021, 77, C800-C800.	0.1	2
774	Supramolecular assemblies involving unconventional non-covalent contacts in pyrazole-based coordination compounds of Co(II) and Cu(II) pyridinedicarboxylates: Antiproliferative evaluation and theoretical studies. Polyhedron, 2022, 224, 116025.	2.2	2

#	Article	IF	Citations
775	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. ChemistrySelect, 2016, 1, 4539-4549.	1.5	1
776	On the Versatility of BH2 X (X=F, Cl, Br, and I) Compounds as Halogen-, Hydrogen-, and Triel-Bond Donors: An Abâ€...Initio Study. ChemPhysChem, 2016, 17, 3150-3150.	2.1	1
777	On the Importance of Nonbonding Donorâ€“Acceptor Interactions Involving PO₂[.] Radicals: An ab Initio Study. ChemPhysChem, 2017, 18, 2191-2196.	2.1	1
778	A combined experimental and computational study of a supramolecular assembly based on cationic zinc(II)-ethanesulfonate. Journal of Molecular Structure, 2020, 1202, 127206.	3.6	1
779	Anion Recognition by Neutral Chalcogen Bonding Receptors: Experimental and Theoretical Investigation. Chemistry - A European Journal, 2020, 26, 4644-4644.	3.3	1
780	Glutamate carboxypeptidase II as a model system for designing hostâ€“guest units: a theoretical approach. Organic and Biomolecular Chemistry, 2021, 19, 7816-7821.	2.8	1
781	Tri- and pentanuclear CuIIâ€“CdII complexes of N2O2 donor ligands with the variation of carboxylate coligands: Structural elucidation and theoretical study. Inorganica Chimica Acta, 2021, 521, 120351.	2.4	1
782	Supramolecular, spectroscopic and computational analysis of weak interactions in some thiosemicarbazones derived from 5-acetylbarbituric acid. Journal of Molecular Structure, 2021, 1245, 131031.	3.6	1
783	Modified-amino acid/peptide pyrimidine analogs: synthesis, structural characterization and DFT studies of N-(pyrimidyl)gabapentine and N-(pyrimidyl)baclofen. New Journal of Chemistry, 0, , .	2.8	1
784	Novel â€˜main-partâ€™ isostructuralism in metal complexes with 1-methylimidazole: crystal structures, energy calculations and magnetic properties. Dalton Transactions, 2021, 50, 17029-17040.	3.3	1
785	Metallophilic interactions in silver(<scp>i</scp>) dicyanoaurate complexes. Dalton Transactions, 2022, , .	3.3	1
786	Combined crystallographic and computational investigation of the solvent disorder present in a new tipiracil hydrochloride methanol solvateâ€“hydrate. CrystEngComm, 0, , .	2.6	1
787	Gold(III) as an effective electrophilic site, namely coinage bond donor: assembly of AuCl₄^{â^’} units into supramolecular anionic polymers. Acta Crystallographica Section A: Foundations and Advances, 2021, 77, C214-C214.	0.1	1
788	Supramolecular Assemblies Based on Ïƒ-hole Interactions. , 2022, , 203-241.		1
789	Hydrogen and halogen bond synergy in the self-assembly of 3,5-dihalo-tyrosines: structural and theoretical insights. CrystEngComm, 2022, 24, 7255-7260.	2.6	1
790	Revision of the Crystal Structure of the Orthorhombic Polymorph of Oxyma: On the Importance of Ï€â€“Hole Interactions and Their Interplay with Hâ€“Bonds. Crystals, 2022, 12, 823.	2.2	1
791	DFT study on CHâ‹¯O, CHÂ·Â·Â·SCN and SÂ·Â·Â· Ï€ interaction energies in three dinuclear mixed valence cobalt(III/II) complexes with secondary diamine ligands having inner N2O2 and outer O4 compartments. Polyhedron, 2022, , 116039.	2.2	1
792	Exploring 3D non-interpenetrated metalâ€“organic framework with malonate-bridged Co(II) coordination polymer: structural elucidation and theoretical study. Phase Transitions, 0, , 1-12.	1.3	0

#	Article	IF	Citations
793	Frontispiece: Adsorption and Quantification of Volatile Organic Compounds (VOCs) by using Hybrid Magnetic Nanoparticles. Chemistry - A European Journal, 2018, 24, .	3.3	0
794	5,5â€²-Dibenzoimidazole as building block for a new 3D Co(II) coordination polymer: A combined EPR and DFT study using UB3LYP model. Polyhedron, 2019, 171, 473-479.	2.2	0
795	Exploitation of the electron deficient outer O4 compartment of a compartmental Schiff base to act as H-bond acceptors in forming a self-assembled dimer of a manganese(III) complex: A joint experimental and theoretical venture. Polyhedron, 2020, 189, 114711.	2.2	0
796	Anion...Ï€, lone pair...Ï€, and F...F interactions in nucleobase derivatives. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C600-C601.	0.3	0
797	CHAPTER 3. Anionâ€“Ï€ Interactions: Theoretical Studies, Supramolecular Chemistry and Catalysis. Monographs in Supramolecular Chemistry, 2016, , 39-97.	0.2	0
798	Crystallographic characterization and elucidation of unconventional interactions of small molecules. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C958-C958.	0.1	0
799	Anionâ€“Ï€ Catalysis. RSC Catalysis Series, 2019, , 122-136.	0.1	0
800	A comparative study of noncovalent interactions in various Ni-compounds containing nitrogen heteroaromatic ligands and pseudohalides: A combined experimental and theoretical studies. Inorganica Chimica Acta, 2022, 531, 120702.	2.4	0
801	Anionâ€“Ï€ Catalysis Enabled by the Mechanical Bond**. Angewandte Chemie, 0, , .	2.0	0
802	Quantification of Aromaticity in Oxocarbons: The Problem of the Fictitious â€œNonaromaticâ€•Reference System. Chemistry - A European Journal, 2002, 8, 433.	3.3	0