Antonio Bauz

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

334 papers	9,283 citations	50 h-index	77 g-index
349 ext. papers	10,639 ext. citations	4.1 avg, IF	6.97 L-index

#	Paper	IF	Citations
334	Enhancing chalcogen bonding by metal coordination.. *Dalton Transactions*, **2022**,	4.3	3
333	Direct conversion of white phosphorus to versatile phosphorus transfer reagents via oxidative onioation.. *Nature Chemistry*, **2022**, 14, 384-391	17.6	2
332	Regium Bonds: A Bridge Between Coordination and Supramolecular Chemistry **2022**, 243-265		
331	Supramolecular Assemblies Based on hole Interactions **2022**, 203-241		
330	On the Importance of Pnictogen and Chalcogen Bonding Interactions in Supramolecular Catalysis. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	9
329	On the Importance of Hole Interactions in Crystal Structures. *Crystals*, **2021**, 11, 1205	2.3	16
328	A homonuclear system with a singlet carbene-type and a nucleophilic phosphorus - the first use in P-heterocyclic synthesis. *Dalton Transactions*, **2021**,	4.3	1
327	Short X N Halogen Bonds With Hexamethylenetetraamine as the Acceptor. *Frontiers in Chemistry*, **2021**, 9, 623595	5	3
326	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	3.4	5
325	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	3.6	4
324	Biological halogen bonds in protein-ligand complexes: a combined QTAIM and NCIPlot study in four representative cases. *Organic and Biomolecular Chemistry*, **2021**, 19, 6858-6864	3.9	2
323	Glutamate carboxypeptidase II as a model system for designing host-guest units: a theoretical approach. *Organic and Biomolecular Chemistry*, **2021**, 19, 7816-7821	3.9	1
322	Spodium bonding in five coordinated Zn(II): a new player in crystal engineering?. *CrystEngComm*, **2021**, 23, 3084-3093	3.3	13
321	Hole spodium bonding in tri-coordinated Hg(II) complexes. *Dalton Transactions*, **2021**, 50, 7545-7553	4.3	3
320	Charge Assisted S/Se Chalcogen Bonds in SAM Riboswitches: A Combined PDB and Study. *ACS Chemical Biology*, **2021**, 16, 1701-1708	4.9	5
319	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	6.1	4
318	Bifunctional Fluorophosphonium Triflates as Intramolecular Frustrated Lewis Pairs: Reversible CO Sequestration and Binding of Carbonyls, Nitriles and Acetylenes. *Chemistry - A European Journal*, **2021**, 27, 13709-13714	4.8	2

317	Importance of Anion-Interactions in RNA GAAA and GGAG Tetraloops: A Combined MD and QM Study. *Journal of Chemical Theory and Computation*, **2021**, 17, 6624-6633	6.4	3
316	Frustrated Lewis Pairs Based on Carbon???Carbon Tetrel Bonds: A DFT Study. *ChemPhysChem*, **2021**, 22, 2478-2483	3.2	0
315	Selenium chalcogen bonds are involved in protein-carbohydrate recognition: a combined PDB and theoretical study. *Physical Chemistry Chemical Physics*, **2021**, 23, 17656-17662	3.6	3
314	Molecular 1,1'-bifunctional mixed-valence P-P compounds, enabled through metal complexation. *Dalton Transactions*, **2021**, 50, 2131-2137	4.3	3
313	Quantifying Intramolecular Halogen Bonds in Nucleic Acids: A Combined Protein Data Bank and Theoretical Study. *ACS Chemical Biology*, **2020**, 15, 1942-1948	4.9	9
312	Spodium Bonds: Noncovalent Interactions Involving Group 12 Elements. *Angewandte Chemie*, **2020**, 132, 17635-17640	3.6	14
311	Spodium Bonds: Noncovalent Interactions Involving Group 12 Elements. *Angewandte Chemie - International Edition*, **2020**, 59, 17482-17487	16.4	70
310	Halogen Bonds in Protein Nucleic Acid Recognition. *Journal of Chemical Theory and Computation*, **2020**, 16, 4744-4752	6.4	12
309	Binuclear and tetranuclear Zn(ii) complexes with thiosemicarbazones: synthesis, X-ray crystal structures, ATP-sensing, DNA-binding, phosphatase activity and theoretical calculations.. *RSC Advances*, **2020**, 10, 12735-12746	3.7	3
308	Halogenhalogen interactions in decahalo-closo-carboranes: CSD analysis and theoretical study. *Physical Chemistry Chemical Physics*, **2020**, 22, 6122-6130	3.6	10
307	Synthesis, X-ray Characterization and Density Functional Theory (DFT) Studies of Two Polymorphs of the Isomer of Tetra--Iodophenyl Tetramethyl Calix[4]pyrrole: On the Importance of Halogen Bonds. *Molecules*, **2020**, 25,	4.8	2
306	Toward N,P-Doped Extended PAHs: A One-Pot Synthesis to Diannulated 1,4,2-Diazaphospholium Triflate Salts. *Journal of Organic Chemistry*, **2020**, 85, 14420-14434	4.2	1
305	Biological promiscuity of a binuclear Cu(II) complex of aminoguanidine Schiff base: DNA binding, anticancer activity and histidine sensing ability of the complex. *New Journal of Chemistry*, **2020**, 44, 7319-7328	3.6	15
304	Ionpair-Interactions favor cell penetration of arginine/tryptophan-rich cell-penetrating peptides. *Biochimica Et Biophysica Acta - Biomembranes*, **2020**, 1862, 183098	3.8	27
303	Halogen and Chalcogen Bond Energies Evaluated Using Electron Density Properties. *ChemPhysChem*, **2020**, 21, 26-31	3.2	39
302	Hole noble gas bonding interactions: Insights from theory and experiment. *Coordination Chemistry Reviews*, **2020**, 404, 213112	23.2	51
301	Intramolecular Spodium Bonds in Zn(II) Complexes: Insights from Theory and Experiment. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	20
300	Supramolecular assemblies involving salt bridges: DFT and X-ray evidence of bipolarity. *CrystEngComm*, **2020**, 22, 8171-8181	3.3	8

299	Novel Pb(II) Complexes: X-Ray Structures, Hirshfeld Surface Analysis and DFT Calculations. *Crystals*, **2020**, 10, 568	2.3	4
298	On the supramolecular properties of neutral, anionic and cationic cadmium complexes harvested from dithiolate–polyamine binary ligand systems. *CrystEngComm*, **2020**, 22, 8023-8035	3.3	3
297	Regium-Bonds Are Involved in Protein-Gold Binding. *Journal of Physical Chemistry Letters*, **2020**, 11, 8259-8263	6.4	10
296	-Hole Interactions Involving Nitro Aromatic Ligands in Protein Structures. *Chemistry - A European Journal*, **2019**, 25, 13436-13443	4.8	15
295	closo-Carboranes as dual CH and BH donors: theoretical study and biological significance. *Physical Chemistry Chemical Physics*, **2019**, 21, 19944-19950	3.6	7
294	Importance of 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	3.5	38
293	Solid-state supramolecular architectures of a series of Hg(II) halide coordination compounds based on hydroxyl-substituted Schiff base ligands. *CrystEngComm*, **2019**, 21, 6301-6312	3.3	8
292	Werner type clathrates involving guest benzoic acid and benzoate in discrete Mn(II) hosts: Experimental and theoretical studies. *Polyhedron*, **2019**, 159, 387-399	2.7	25
291	Tetrel bonding interactions at work: Impact on tin and lead coordination compounds. *Coordination Chemistry Reviews*, **2019**, 384, 107-125	23.2	106
290	H-Bonded anion-anion complexes in fentanyl citrate polymorphs and solvates. *Chemical Communications*, **2019**, 55, 115-118	5.8	22
289	Formation of an imidazoliumyl-substituted [(L)P] tetracation and transition metal mediated fragmentation and insertion reaction (L = NHC). *Chemical Science*, **2019**, 10, 6868-6875	9.4	13
288	Synchronized On/Off Switching of Four Binding Sites for Water in a Molecular Solomon Link. *Angewandte Chemie*, **2019**, 131, 8137-8141	3.6	3
287	An inorganic-organic hybrid supramolecular framework based on the [MoO] cluster and cobalt complex of aspartic acid: X-ray structure and DFT study. *Acta Crystallographica Section C, Structural Chemistry*, **2019**, 75, 469-477	0.8	9
286	Synchronized On/Off Switching of Four Binding Sites for Water in a Molecular Solomon Link. *Angewandte Chemie - International Edition*, **2019**, 58, 8053-8057	16.4	13
285	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	2.7	6
284	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	4.3	3
283	The role of 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	0.8	9
282	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	2.7	6

281	Observation of an anion?anion interaction in a square planar copper(II) Schiff base complex: DFT study and CSD analysis. *Inorganica Chimica Acta*, **2019**, 487, 465-472	2.7	8
280	Synthesis, characterization and DFT study on two copper(II) complexes with a naphthalene-based Schiff base: Examples of stronger chelate chelate interactions than those reported for classical complexes. *Polyhedron*, **2019**, 157, 487-494	2.7	10
279	Anion Interactions in Hollow Crystals of a Copper(II)-Cyamelurate Coordination Complex. *Crystal Growth and Design*, **2018**, 18, 2636-2644	3.5	11
278	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	2.7	12
277	Non-covalent tetrel bonding interactions in hemidirectional lead(II) complexes with nickel(II)-salen type metalloligands. *New Journal of Chemistry*, **2018**, 42, 6062-6076	3.6	30
276	Regium- bonds: An Unexplored Link between Noble Metal Nanoparticles and Aromatic Surfaces. *Chemistry - A European Journal*, **2018**, 24, 7228-7234	4.8	51
275	Pb?X (X = N, S, I) tetrel bonding interactions in Pb(II) complexes: X-ray characterization, Hirshfeld surfaces and DFT calculations. *CrystEngComm*, **2018**, 20, 2812-2821	3.3	56
274	Copper(II) polyamine chelates as efficient receptors for acyclovir: syntheses, crystal structures and dft study. *Polyhedron*, **2018**, 145, 218-226	2.7	5
273	Formation of a water-mediated assembly of two neutral copper(II) Schiff base fragments with a Cu2(NCS)4 moiety: exploration of non-covalent CH?(bimetallo ring) interactions. *CrystEngComm*, **2018**, 20, 1679-1689	3.3	22
272	Methylene spacer regulated variation in conformation of tetradentate N2O2 donor Schiff bases trapped in manganese(III) complexes. *CrystEngComm*, **2018**, 20, 1077-1086	3.3	18
271	Synthesis, Substitution, and Oxidation of Imidazole-2-thione Based Tricyclic 1,4-Dihydro-1,4-diphosphinines. *European Journal of Inorganic Chemistry*, **2018**, 2018, 904-916	2.3	8
270	Screening polymorphism in a Ni(II) metal organic framework: experimental observations, Hirshfeld surface analyses and DFT studies. *CrystEngComm*, **2018**, 20, 746-754	3.3	55
269	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	3.3	33
268	Synergistic Anion- -Catalysis on Stacked Foldamers. *Journal of the American Chemical Society*, **2018**, 140, 4884-4892	16.4	55
267	Molecular electrostatic potential and "atoms-in-molecules" analyses of the interplay between hole and lone pair X-H metal interactions. *Journal of Computational Chemistry*, **2018**, 39, 458-463	3.5	18
266	Anion-reliant structural versatility of novel cadmium(II) complexes: Synthesis, crystal structures, photoluminescence properties and exploration of unusual O S chalcogen bonding involving thiocyanate coligand. *Inorganica Chimica Acta*, **2018**, 469, 189-196	2.7	14
265	On the importance of Pb?X (X = O, N, S, Br) tetrel bonding interactions in a series of tetra- and hexa-coordinated Pb(II) compounds. *CrystEngComm*, **2018**, 20, 5033-5044	3.3	27
264	Regium- vs Cation- Interactions in M2 and MCl (M = Cu, Ag and Au) Complexes with Small Aromatic Systems: An ab Initio Study. *Inorganics*, **2018**, 6, 64	2.9	21

263	Chalcogen 'like-like' Interactions Involving Trisulphide and Triselenide Compounds: A Combined CSD and Ab Initio Study. *Molecules*, **2018**, 23,	4.8	21
262	Coordination Polymers Based on Phthalic Acid and Aminopyrazine Ligands: On the Importance of N?H Interactions. *Polymers*, **2018**, 10,	4.5	12
261	Synthesis of Multinuclear Zn(II) Complexes Involving 8-Aminoquinoline- Based Schiff-Base Ligand: Structural Diversity, DNA Binding Studies and Theoretical Calculations.. *ChemistrySelect*, **2018**, 3, 7697-7706	1.8	5
260	Crystal structures of N6-modified-aminoacid/peptide nucleobase analogs: hybrid adenine glycine and adenine glycylglycine molecules. *New Journal of Chemistry*, **2018**, 42, 14742-14750	3.6	7
259	Quantifying conventional CH?(aryl) and unconventional CH?(chelate) interactions in dinuclear Cu(II) complexes: experimental observations, Hirshfeld surface and theoretical DFT study. *New Journal of Chemistry*, **2018**, 42, 10202-10213	3.6	50
258	A Strategy to Synthesize Molecular Knots and Links Using the Hydrophobic Effect. *Journal of the American Chemical Society*, **2018**, 140, 12442-12450	16.4	54
257	One pot synthesis of two cobalt(iii) Schiff base complexes with chelating pyridyltetrazolate and exploration of their bio-relevant catalytic activities.. *RSC Advances*, **2018**, 8, 28216-28237	3.7	20
256	Bipolar behaviour of salt-bridges: a combined theoretical and crystallographic study. *New Journal of Chemistry*, **2018**, 42, 12134-12142	3.6	14
255	A comparative experimental and theoretical investigation of hydrogen-bond, halogen-bond and interactions in the solid-state supramolecular assembly of 2- and 4-formylphenyl arylsulfonates. *Acta Crystallographica Section C, Structural Chemistry*, **2018**, 74, 816-829	0.8	6
254	Heteronuclear cobalt(iii)/sodium complexes with salen type compartmental Schiff base ligands: methylene spacer regulated variation in nuclearity. *Dalton Transactions*, **2018**, 47, 331-347	4.3	45
253	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	2.7	11
252	H-Bonded anion-anion complex trapped in a squaramido-based receptor. *Chemical Communications*, **2018**, 54, 1841-1844	5.8	28
251	Polymorphism in secondary squaramides: on the importance of interactions involving the four membered ring. *CrystEngComm*, **2018**, 20, 237-244	3.3	10
250	Structure guided or structure guiding? Mixed carbon/hydrogen bonding in a bis-Schiff base of N-allyl isatin. *CrystEngComm*, **2018**, 20, 150-154	3.3	12
249	A versatile quinoxaline derivative serves as a colorimetric sensor for strongly acidic pH. *Dalton Transactions*, **2018**, 47, 17077-17085	4.3	13
248	Hole halogen bonding interactions in a mixed valence cobalt(III/II) complex and anti-electrostatic hydrogen bonding interaction in a cobalt(III) complex: a theoretical insight. *CrystEngComm*, **2018**, 20, 7281-7292	3.3	22
247	A versatile chemosensor for the detection of Al and picric acid (PA) in aqueous solution. *Dalton Transactions*, **2018**, 47, 15907-15916	4.3	16
246	S???Sn Tetrel Bonds in the Activation of Peroxisome Proliferator-Activated Receptors (PPARs) by Organotin Molecules. *Chemistry - A European Journal*, **2018**, 24, 16582-16587	4.8	27

245	Multicomponent Supramolecular Assemblies of Melamine and α-Hydroxycarboxylic Acids: Understanding the Hydrogen Bonding Patterns and Their Physicochemical Consequences. *Crystal Growth and Design*, **2018**, 18, 6786-6800	3.5	16
244	Bioactive Heterometallic Cu-Zn Complexes with Potential Biomedical Applications. *ACS Omega*, **2018**, 3, 13343-13353	3.9	6
243	Surface-grafted lanthanoid complexes of the tungstosilicate polyanion [SiWO]: a synthetic, structural and computational investigation. *Acta Crystallographica Section C, Structural Chemistry*, **2018**, 74, 1300-1309	0.8	14
242	Tetrel Bonding Interactions in Perchlorinated Cyclopenta- and Cyclohexatetrelanes: A Combined DFT and CSD Study. *Molecules*, **2018**, 23,	4.8	9
241	Effect of temperature and ligand protonation on the electronic ground state in Cu(ii) polymers having unusual secondary interactions: a magnetic and catechol oxidase study. *Dalton Transactions*, **2018**, 47, 16102-16118	4.3	9
240	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	5.5	3
239	Joining of trinuclear (CuL)2M (M = MnII and CdII) nodes by 1,3- and 1,4-benzenedicarboxylate linkers: positional isomeric effect on co-crystallization. *CrystEngComm*, **2018**, 20, 6490-6501	3.3	13
238	Cu(II)N6-Alkyladenine Complexes: Synthesis, X-ray Characterization and Magnetic Properties. *Magnetochemistry*, **2018**, 4, 24	3.1	2
237	Intramolecular Noncovalent Carbon Bonding Interaction Stabilizes the cis Conformation in Acylhydrazones. *ChemPlusChem*, **2018**, 83, 881-885	2.8	18
236	Boron triel bonding: a weak electrostatic interaction lacking electron-density descriptors. *Physical Chemistry Chemical Physics*, **2018**, 20, 24192-24200	3.6	31
235	Synthesis, structural features, antibacterial behaviour and theoretical investigation of two new manganese(III) Schiff base complexes. *Polyhedron*, **2018**, 151, 407-416	2.7	6
234	Remote Control of Anion-Catalysis on Fullerene-Centered Catalytic Triads. *Angewandte Chemie - International Edition*, **2018**, 57, 10883-10887	16.4	25
233	Remote Control of Anion Catalysis on Fullerene-Centered Catalytic Triads. *Angewandte Chemie*, **2018**, 130, 11049-11053	3.6	18
232	Lone pair vs. hole interactions in bromine head-containing oxacalix[2]arene[2]triazines. *CrystEngComm*, **2018**, 20, 3251-3257	3.3	14
231	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	3.6	4
230	Hydrogen bonding versus interactions: their key competition in sildenafil solvates. *CrystEngComm* , **2018**, 20, 4526-4530	3.3	5
229	Pseudohalides regulated diverse helicity in copper(II) coordination polymers derived from a bis(aminoethoxy) ligand. *Polyhedron*, **2017**, 124, 262-274	2.7	3
228	Melamine-mediated self-assembly of a Cu(II)ethylmalonate complex assisted by and anti-electrostatic H-bonding interactions. *Journal of Coordination Chemistry*, **2017**, 70, 463-474	1.6	7

227	NO- anions can act as Lewis acid in the solid state. *Nature Communications*, **2017**, 8, 14522	17.4	55
226	Carbodiphosphorane mediated synthesis of a triflyloxyphosphonium dication and its reactivity towards nucleophiles. *Chemical Communications*, **2017**, 53, 2954-2957	5.8	12
225	Introducing Supramolecular Interactions into Robust Bis(tetrabromocatecholate) Chelated Manganese(III) Systems and Biomimetic Catalytic Activity. *ChemistrySelect*, **2017**, 2, 2094-2105	1.8	9
224	Synthesis and crystal structures of three new lead(II) isonicotinoylhydrazone derivatives: Anion controlled nuclearity and dimensionality. *Inorganica Chimica Acta*, **2017**, 461, 192-205	2.7	26
223	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	2.7	3
222	Competition between lone pair-, halogen- and triel bonding interactions involving BX3 (X = F, Cl, Br and I) compounds: an ab initio study. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	25
221	Unraveling the dual character of sulfur atoms in a series of Hg(II) coordination polymers containing bis(4-pyridyl)disulfide. *CrystEngComm*, **2017**, 19, 1974-1981	3.3	11
220	On the Importance of Hole Beryllium Bonds: Theoretical Study and Biological Implications. *Chemistry - A European Journal*, **2017**, 23, 5375-5380	4.8	18
219	A highly selective ONOFF probe for colorimetric and fluorometric sensing of Cu2+ in water. *RSC Advances*, **2017**, 7, 11312-11321	3.7	21
218	Molecular and crystalline architectures based on HgI2: from metallamacrocycles to coordination polymers. *CrystEngComm*, **2017**, 19, 3322-3330	3.3	6
217	Selective and Reversible Fluoride Complexation from Water by a Cyclic Tri(phosphonio)methanide Dication. *Angewandte Chemie - International Edition*, **2017**, 56, 7907-7911	16.4	12
216	A combined crystallographic and theoretical study of weak intermolecular interactions in crystalline squaric acid esters and amides. *CrystEngComm*, **2017**, 19, 3071-3077	3.3	5
215	Isolation of Azadiphosphiridines and Diphosphenimines by Cycloaddition of Azides and a Cationic Diphosphene. *Angewandte Chemie - International Edition*, **2017**, 56, 6218-6222	16.4	6
214	Selective and Reversible Fluoride Complexation from Water by a Cyclic Tri(phosphonio)methanide Dication. *Angewandte Chemie*, **2017**, 129, 8015-8019	3.6	2
213	Supramolecular nanotubes based on halogen bonding interactions: cooperativity and interaction with small guests. *Physical Chemistry Chemical Physics*, **2017**, 19, 12936-12941	3.6	24
212	Exploring 3D non-interpenetrated metalorganic framework with malonate-bridged Co(II) coordination polymer: structural elucidation and theoretical study. *Phase Transitions*, **2017**, 1-12	1.3	
211	The Mouse in a Trap: Observation of a C(sp3)FCF(sp3) Interaction in a Discrete CFC Pair by the Crystal Sponge Method. *Crystal Growth and Design*, **2017**, 17, 3611-3615	3.5	10
210	The roles of H-bonding, stacking, and antiparallel CO ? 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	3.1	6

209	On the Importance of Nonbonding Donor-Acceptor Interactions Involving PO Radicals: An ab Initio Study. *ChemPhysChem*, **2017**, 18, 2191-2196	3.2	1
208	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	3.4	12
207	Synthesis, Characterization, DFT Study, Catechol Oxidase and Phenoxazinone Synthase Like Activities of Two New Manganese(IV) Schiff Base Complexes. *ChemistrySelect*, **2017**, 2, 2975-2984	1.8	16
206	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	4.3	18
205	Mononuclear and dinuclear trimethylplatinum(IV) iodide complexes of 3-substituted pyridines. *New Journal of Chemistry*, **2017**, 41, 3498-3507	3.6	3
204	Hole interactions at work: crystal engineering with nitro-derivatives. *CrystEngComm*, **2017**, 19, 1933-1937	3.3	48
203	Estimation of conventional C-H (arene), unconventional C-H (chelate) and C-H (thiocyanate) interactions in hetero-nuclear nickel(ii)-cadmium(ii) complexes with a compartmental Schiff base. *Dalton Transactions*, **2017**, 46, 5384-5397	4.3	43
202	Synthesis and supramolecular self-assembly of thioxothiazolidinone derivatives driven by H-bonding and diverse Hole interactions: A combined experimental and theoretical analysis. *Journal of Molecular Structure*, **2017**, 1139, 209-221	3.4	8
201	Ambiguous reactivity of Li/Cl phosphinidenoid complexes under redox conditions - a novel dichotomy in phosphorus chemistry. *Chemical Communications*, **2017**, 53, 933-936	5.8	2
200	X-ray Crystal Structure of a Metalled Double-Helix Generated by Infinite and Consecutive C*-Ag -C* (C*:N -Hexylcytosine) Base Pairs through Argentophilic and Hydrogen Bond Interactions. *Chemistry - A European Journal*, **2017**, 23, 2103-2108	4.8	32
199	Solid-state inclusion of C60 and C70 in a co-polymer induced by metal ligand coordination of a Zn porphyrin cage with a bis-pyridyl perylene derivative. *CrystEngComm*, **2017**, 19, 4911-4919	3.3	12
198	Observation of 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	2.7	29
197	Concurrent aerogen bonding and lone pair/anion- interactions in the stability of organoxenon derivatives: a combined CSD and ab initio study. *Physical Chemistry Chemical Physics*, **2017**, 19, 30063-30068	2.6	25
196	Cooperative influence of pseudohalides and ligand backbone of Schiff-bases on nuclearity and stereochemistry of cobalt(iii) complexes: experimental and theoretical investigation. *Dalton Transactions*, **2017**, 46, 15257-15268	4.3	13
195	Donor-acceptor interactions in tri(phosphonio)methanide dications [(PhP)CP(X)Ph] (X = H, Me, CN, NCS, OH, Cl, OTf, F). *Dalton Transactions*, **2017**, 46, 15503-15511	4.3	4
194	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	1.8	30
193	Substituent Effects in Multivalent Halogen Bonding Complexes: A Combined Theoretical and Crystallographic Study. *Molecules*, **2017**, 23,	4.8	6
192	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	4.2	7

191	A polynuclear and two dinuclear copper(II) Schiff base complexes: Synthesis, characterization, self-assembly, magnetic property and DFT study. *Polyhedron*, **2017**, 137, 332-346	2.7	17
190	Nuclearity versus oxidation state in the catalytic efficiency of MnII/III azo Schiff base complexes: computational study on supramolecular interactions and phenoxazinone synthase-like activity. *New Journal of Chemistry*, **2017**, 41, 11607-11618	3.6	10
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