

Antonio Bauz

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334
papers

9,283
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50
h-index

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349
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L-index

#	Paper	IF	Citations
334	Tetrel-bonding interaction: rediscovered supramolecular force?. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 12317-21	16.4	473
333	The bright future of unconventional π -hole interactions. <i>ChemPhysChem</i> , 2015 , 16, 2496-517	3.2	458
332	Aerogen Bonding Interaction: A New Supramolecular Force?. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 7340-3	16.4	239
331	On the Reliability of Pure and Hybrid DFT Methods for the Evaluation of Halogen, Chalcogen, and Pnicogen Bonds Involving Anionic and Neutral Electron Donors. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 5201-10	6.4	204
330	Halogen bonding versus chalcogen and pnicogen bonding: a combined Cambridge structural database and theoretical study. <i>CrystEngComm</i> , 2013 , 15, 3137-3144	3.3	187
329	Tetrel Bonding Interactions. <i>Chemical Record</i> , 2016 , 16, 473-87	6.6	145
328	A thorough anion- π interaction study in biomolecules: on the importance of cooperativity effects. <i>Chemical Science</i> , 2016 , 7, 1038-1050	9.4	122
327	Tetrel bonding interactions at work: Impact on tin and lead coordination compounds. <i>Coordination Chemistry Reviews</i> , 2019 , 384, 107-125	23.2	106
326	Directionality of π -holes in nitro compounds. <i>Chemical Communications</i> , 2015 , 51, 1491-3	5.8	106
325	Unprecedented structural variations in trinuclear mixed valence Co(II/III) complexes: theoretical studies, pnicogen bonding interactions and catecholase-like activities. <i>Dalton Transactions</i> , 2015 , 44, 3862-76	4.3	99
324	Pnicogen- π complexes: theoretical study and biological implications. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 14061-6	3.6	93
323	Experimental and Computational Study of Counterintuitive $\text{ClO}_4^- \cdots \text{ClO}_4^-$ Interactions and the Interplay between π - π and Anion- π Interactions. <i>Crystal Growth and Design</i> , 2014 , 14, 5812-5821	3.5	92
322	Rationalization of Noncovalent Interactions within Six New MII/8-Aminoquinoline Supramolecular Complexes (MII = Mn, Cu, and Cd): A Combined Experimental and Theoretical DFT Study. <i>Crystal Growth and Design</i> , 2015 , 15, 1351-1361	3.5	88
321	A combined theoretical and Cambridge Structural Database study of π -hole pnicogen bonding complexes between electron rich molecules and both nitro compounds and inorganic bromides (YO_2Br , Y = N, P, and As). <i>Journal of Physical Chemistry A</i> , 2014 , 118, 2827-34	2.8	86
320	π -hole aerogen bonding interactions. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 24748-53	3.6	84
319	Design of Lead(II) Metal-Organic Frameworks Based on Covalent and Tetrel Bonding. <i>Chemistry - A European Journal</i> , 2015 , 21, 17951-8	4.8	84
318	Substituent effects in halogen bonding complexes between aromatic donors and acceptors: a comprehensive ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 20371-9	3.6	82

317	Towards design strategies for anion-π interactions in crystal engineering. <i>CrystEngComm</i> , 2016 , 18, 10-23	3.3	80
316	Small cycloalkane (CN) ₂ C-C(CN) ₂ structures are highly directional non-covalent carbon-bond donors. <i>Chemistry - A European Journal</i> , 2014 , 20, 10245-8	4.8	79
315	3-Picoline mediated self-assembly of M(II)-malonate complexes (M = Ni/Co/Mn/Mg/Zn/Cu) assisted by various weak forces involving lone pair-π and anion-π-hole interactions. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 14713-26	3.4	77
314	Tetrel-Bonding Interaction: Rediscovered Supramolecular Force?. <i>Angewandte Chemie</i> , 2013 , 125, 12543-12547	3.1	77
313	A combined experimental and theoretical investigation on the role of halide ligands on the catecholase-like activity of mononuclear nickel(II) complexes with a phenol-based tridentate ligand. <i>Inorganic Chemistry</i> , 2013 , 52, 13442-52	5.1	76
312	Non-covalent sp ³ carbon bonding with ArCF ₃ is analogous to CH-π interactions. <i>Chemical Communications</i> , 2014 , 50, 12626-9	5.8	75
311	Hydrogen Bond, π and CH-π Interactions Governing the Supramolecular Assembly of Some Hydrazone Ligands and Their MnII Complexes: Structural and Theoretical Interpretation. <i>European Journal of Inorganic Chemistry</i> , 2015 , 2015, 1958-1972	2.3	72
310	On the directionality of anion-π interactions. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 5696-702	3.6	72
309	Exploration of CH-π interactions involving the π-system of pseudohalide coligands in metal complexes of a Schiff-base ligand. <i>CrystEngComm</i> , 2015 , 17, 4680-4690	3.3	71
308	Use of metalloligands [CuL] (H ₂ L = salen type di-Schiff bases) in the formation of heterobimetallic copper(II)-uranyl complexes: photophysical investigations, structural variations, and theoretical calculations. <i>Inorganic Chemistry</i> , 2013 , 52, 7508-23	5.1	71
307	Spodium Bonds: Noncovalent Interactions Involving Group 12 Elements. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 17482-17487	16.4	70
306	Relation between the catalytic efficiency of the synthetic analogues of catechol oxidase with their electrochemical property in the free state and substrate-bound state. <i>Inorganic Chemistry</i> , 2014 , 53, 8257-69	5.1	65
305	Concurrent agostic and tetrel bonding interactions in lead(II) complexes with an isonicotinohydrazide based ligand and several anions. <i>Dalton Transactions</i> , 2016 , 45, 4965-9	4.3	63
304	RCH ₃ ⋯O Interactions in Biological Systems: Are They Trifurcated H-Bonds or Noncovalent Carbon Bonds?. <i>Crystals</i> , 2016 , 6, 26	2.3	63
303	On the importance of tetrel bonding interactions in lead(II) complexes with (iso)nicotinohydrazide based ligands and several anions. <i>Dalton Transactions</i> , 2016 , 45, 10708-16	4.3	60
302	Computational study of anion recognition based on tetrel and hydrogen bonding interaction by calix[4]pyrrole derivatives. <i>Computational and Theoretical Chemistry</i> , 2014 , 1038, 67-70	2	60
301	pH Dependent Formation of Unprecedented Water-Bromide Cluster in the Bromide Salts of PTP Assisted by Anion-π Interactions: Synthesis, Structure, and DFT Study. <i>Crystal Growth and Design</i> , 2014 , 14, 747-755	3.5	58
300	Pb-X (X = N, S, I) tetrel bonding interactions in Pb(II) complexes: X-ray characterization, Hirshfeld surfaces and DFT calculations. <i>CrystEngComm</i> , 2018 , 20, 2812-2821	3.3	56

- 299 NO⁻ anions can act as Lewis acid in the solid state. *Nature Communications*, **2017**, 8, 14522 17.4 55
- 298 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
- 297 Synergistic Anion- π -Catalysis on π -Stacked Foldamers. *Journal of the American Chemical Society*, **2018**, 140, 4884-4892 16.4 55
- 296 Syntheses, structures, properties and DFT study of hybrid inorganic-organic architectures constructed from trinuclear lanthanide frameworks and Keggin-type polyoxometalates. *Dalton Transactions*, **2014**, 43, 1906-16 4.3 55
- 295 Theoretical Study on the Dual Behavior of XeO₃ and XeF₄ toward Aromatic Rings: Lone Pair- π versus Aerogen- π Interactions. *ChemPhysChem*, **2015**, 16, 3625-30 3.2 55
- 294 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, 8502-13 5.1 55
- 293 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
- 292 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 2.7 53
- 291 The influence of H-bonding on the 'ambidentate' coordination behaviour of the thiocyanate ion to Cd(II): a combined experimental and theoretical study. *Dalton Transactions*, **2014**, 43, 8007-15 4.3 53
- 290 Importance of R-CF₃...O Tetrel Bonding Interactions in Biological Systems. *Journal of Physical Chemistry A*, **2017**, 121, 5371-5376 2.8 52
- 289 Regium- π Bonds: An Unexplored Link between Noble Metal Nanoparticles and Aromatic Surfaces. *Chemistry - A European Journal*, **2018**, 24, 7228-7234 4.8 51
- 288 π -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, 1608-14 3.2 51
- 287 Salt-bridge(π)- π interactions at work: associative interactions of π -stacked anion- π Cu(II)-malonate- π -aminopyridine-hexafluoridophosphate ternary system. *CrystEngComm*, **2013**, 15, 686-696 3.3 51
- 286 π -Hole noble gas bonding interactions: Insights from theory and experiment. *Coordination Chemistry Reviews*, **2020**, 404, 213112 23.2 51
- 285 π -Hole Interactions Involving Nitro Compounds: Directionality of Nitrate Esters. *Crystal Growth and Design*, **2016**, 16, 5520-5524 3.5 51
- 284 Quantifying conventional C π ... π (aryl) and unconventional C π ... π (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
- 283 π -hole interactions at work: crystal engineering with nitro-derivatives. *CrystEngComm*, **2017**, 19, 1933-1937 3.3 48
- 282 A crystalline sponge based on dispersive forces suitable for X-ray structure determination of included molecular guests. *Chemical Science*, **2015**, 6, 5466-5472 9.4 48

281	MIIMalonate Complexes (M = Mg, Cu, Ni and Co) Characterized by Layered Structures: Experimental Observation, Hirshfeld Surface Analysis and Theoretical Study. <i>European Journal of Inorganic Chemistry</i> , 2013 , 2013, 4679-4685	2.3	48
280	Nature of noncovalent carbon-bonding interactions derived from experimental charge-density analysis. <i>ChemPhysChem</i> , 2015 , 16, 2530-3	3.2	47
279	Differences in nuclearity, molecular shapes, and coordination modes of azide in the complexes of Cd(II) and Hg(II) with a "metalloligand" [CuL] (H ₂ L = N,N'-bis(salicylidene)-1,3-propanediamine): characterization in solid and in solutions, and theoretical calculations. <i>Inorganic Chemistry</i> , 2012 , 51, 12407-18	5.1	47
278	A Schiff base platform: structures, sensing of Zn(ii) and PPI in aqueous medium and anticancer activity. <i>Dalton Transactions</i> , 2017 , 46, 9498-9510	4.3	46
277	1,1,2,2-Tetracyanocyclopropane (TCCP) as supramolecular synthon. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 1693-8	3.6	45
276	Heteronuclear cobalt(iii)/sodium complexes with salen type compartmental Schiff base ligands: methylene spacer regulated variation in nuclearity. <i>Dalton Transactions</i> , 2018 , 47, 331-347	4.3	45
275	Crystal engineering with coordination compounds of NiII, CoII, and CrIII bearing dipicolinic acid driven by the nature of the noncovalent interactions. <i>CrystEngComm</i> , 2014 , 16, 5352	3.3	44
274	Supramolecularly Regulated Ligands for Asymmetric Hydroformylations and Hydrogenations. <i>Chemistry - A European Journal</i> , 2015 , 21, 11417-26	4.8	44
273	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. <i>Dalton Transactions</i> , 2017 , 46, 5384-5397	4.3	43
272	A new family of Ni ₄ and Ni ₆ aggregates from the self-assembly of [Ni ₂] building units: role of carboxylate and carbonate bridges. <i>Inorganic Chemistry</i> , 2015 , 54, 4709-23	5.1	39
271	Exploring the coordinative adaptation and molecular shapes of trinuclear CuM(II) (M = Zn/Cd) complexes derived from salen type Schiff bases: structural and theoretical studies. <i>Dalton Transactions</i> , 2016 , 45, 5730-40	4.3	39
270	Halogen and Chalcogen Bond Energies Evaluated Using Electron Density Properties. <i>ChemPhysChem</i> , 2020 , 21, 26-31	3.2	39
269	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. <i>Crystal Growth and Design</i> , 2019 , 19, 5869-5881	3.5	38
268	Metal...organic and supramolecular lead(II) networks assembled from isomeric nicotinoylhydrazone blocks: the effects of ligand geometry and counter-ion on topology and supramolecular assembly. <i>CrystEngComm</i> , 2016 , 18, 5375-5385	3.3	38
267	Benzyl Dihydrazone versus Thiosemicarbazone Schiff Base: Effects on the Supramolecular Arrangement of Cobalt Thiocyanate Complexes and the Generation of CoN ₆ and CoN ₄ S ₂ Coordination Spheres. <i>European Journal of Inorganic Chemistry</i> , 2017 , 2017, 4763-4772	2.3	37
266	Charge-assisted triel bonding interactions in solid state chemistry: A combined computational and crystallographic study. <i>Chemical Physics Letters</i> , 2016 , 666, 73-78	2.5	36
265	Cationic 5-phosphonio-substituted N-heterocyclic carbenes. <i>Dalton Transactions</i> , 2016 , 45, 11384-96	4.3	36
264	Influence of ring size on the strength of carbon bonding complexes between anions and perfluorocycloalkanes. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 19192-7	3.6	35

263	Fluorescent sensing of Al ³⁺ by benzophenone based Schiff base chemosensor and live cell imaging applications: Impact of keto-enol tautomerism. <i>Sensors and Actuators B: Chemical</i> , 2017 , 239, 1194-1204	8.5	35
262	The role of unconventional stacking interactions in the supramolecular assemblies of Hg(II) coordination compounds. <i>CrystEngComm</i> , 2016 , 18, 9056-9066	3.3	34
261	Recurrent supramolecular motifs in discrete complexes and coordination polymers based on mercury halides: prevalence of chelate ring stacking and substituent effects. <i>CrystEngComm</i> , 2018 , 20, 1065-1076	3.3	33
260	Crystal engineering with coordination compounds of 2,6-dicarboxy-4-hydroxypyridine and 9-aminoacridine fragments driven by different nature of the face-to-face π -stacking. <i>CrystEngComm</i> , 2014 , 16, 1359-1377	3.3	33
259	The development of a promising photosensitive Schottky barrier diode using a novel Cd(II) based coordination polymer. <i>Dalton Transactions</i> , 2017 , 46, 13531-13543	4.3	33
258	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. <i>Chemistry - A European Journal</i> , 2017 , 23, 2103-2108	4.8	32
257	Competition between Halogen Bonding and π -Hole Interactions Involving Various Donors: The Role of Dispersion Effects. <i>ChemPhysChem</i> , 2015 , 16, 3108-13	3.2	32
256	Catecholase activity, DNA binding and cytotoxicity studies of a Cu(II) complex of a pyridoxal schiff base: synthesis, X-ray crystal structure, spectroscopic, electrochemical and theoretical studies. <i>RSC Advances</i> , 2016 , 6, 86851-86861	3.7	32
255	A combined experimental and computational study on supramolecular assemblies in hetero-tetranuclear nickel(II)-cadmium(II) complexes with NO-donor compartmental Schiff bases. <i>Dalton Transactions</i> , 2016 , 45, 15048-15059	4.3	32
254	Long-range effects in anion- π interactions: their crucial role in the inhibition mechanism of Mycobacterium tuberculosis malate synthase. <i>Chemistry - A European Journal</i> , 2014 , 20, 6985-90	4.8	31
253	Boron triel bonding: a weak electrostatic interaction lacking electron-density descriptors. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 24192-24200	3.6	31
252	A Combined Experimental and Theoretical Study on the Formation of a Cyclic Tetrameric Water Cluster and a Similar Type of Cyclic Cluster in Copper(II) Schiff Base Complexes. <i>ChemistrySelect</i> , 2017 , 2, 9336-9343	1.8	30
251	Non-covalent tetrel bonding interactions in hemidirectional lead(II) complexes with nickel(II)-salen type metalloligands. <i>New Journal of Chemistry</i> , 2018 , 42, 6062-6076	3.6	30
250	Understanding the forces that govern packing: a density functional theory and structural investigation of anion- π and nonclassical C-H \cdots anion interactions. <i>Inorganic Chemistry</i> , 2012 , 51, 10334-40	5.1	30
249	On the importance of unprecedented lone pair-salt bridge interactions in Cu(II)-malonate-2-amino-5-chloropyridine-perchlorate ternary system. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 5802-11	2.8	30
248	Observation of π -hole interactions in the solid state structures of three new copper(II) complexes with a tetradentate N ₄ donor Schiff base: Exploration of their cytotoxicity against MDA-MB 468 cells. <i>Polyhedron</i> , 2017 , 123, 334-343	2.7	29
247	Synthesis, crystal structure, antimicrobial screening and density functional theory calculation of nickel(II), cobalt(II) and zinc(II) mononuclear Schiff base complexes. <i>Inorganica Chimica Acta</i> , 2015 , 425, 211-220	2.7	29
246	Synthesis, structural characterization, theoretical calculations and catecholase mimetic activity of manganese-Schiff base complexes. <i>Polyhedron</i> , 2014 , 75, 40-49	2.7	29

245	On the importance of non covalent interactions in the structure of coordination Cu(II) and Co(II) complexes of pyrazine- and pyridine-dicarboxylic acid derivatives: experimental and theoretical views. <i>CrystEngComm</i> , 2014 , 16, 6149-6158	3.3	29
244	Analysis of the contribution of the acidity of the s-tetrazine ring in the crystal packing of coordination polymers. <i>CrystEngComm</i> , 2013 , 15, 3031	3.3	29
243	Observation of novel oxygen-oxygen interaction in supramolecular assembly of cobalt(III) Schiff base complexes: a combined experimental and computational study. <i>RSC Advances</i> , 2015 , 5, 73028-73039	3.7	28
242	Synthesis, X-ray characterization, DFT calculations and Hirshfeld surface analysis studies of carbohydrazone based on Zn(II) complexes. <i>CrystEngComm</i> , 2016 , 18, 102-112	3.3	28
241	Molecular recognition of nucleotides in water by scorpion-type receptors based on nucleobase discrimination. <i>Chemistry - A European Journal</i> , 2014 , 20, 3730-41	4.8	28
240	On the importance of anion-π interactions in the mechanism of sulfide:quinone oxidoreductase. <i>Chemistry - an Asian Journal</i> , 2013 , 8, 2708-13	4.5	28
239	Aerogen Bonding Interaction: A New Supramolecular Force?. <i>Angewandte Chemie</i> , 2015 , 127, 7448-7451	3.6	28
238	Substituent effects in cation-π interactions revisited: a general approach based on intrinsic properties of the arenes. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 1322-6	3.6	28
237	Asymmetric Hydrogenation of Seven-Membered C=N-containing Heterocycles and Rationalization of the Enantioselectivity. <i>Chemistry - A European Journal</i> , 2016 , 22, 10607-13	4.8	28
236	H-Bonded anion-anion complex trapped in a squaramido-based receptor. <i>Chemical Communications</i> , 2018 , 54, 1841-1844	5.8	28
235	On the importance of Pb-X (X = O, N, S, Br) tetrel bonding interactions in a series of tetra- and hexa-coordinated Pb(II) compounds. <i>CrystEngComm</i> , 2018 , 20, 5033-5044	3.3	27
234	Is the use of diffuse functions essential for the properly description of noncovalent interactions involving anions?. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 2651-5	2.8	27
233	Ion-pair-π interactions favor cell penetration of arginine/tryptophan-rich cell-penetrating peptides. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020 , 1862, 183098	3.8	27
232	Electrostatically enhanced FF interactions through hydrogen bonding, halogen bonding and metal coordination: an ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 20381-8	3.6	27
231	Sn Tetrel Bonds in the Activation of Peroxisome Proliferator-Activated Receptors (PPARs) by Organotin Molecules. <i>Chemistry - A European Journal</i> , 2018 , 24, 16582-16587	4.8	27
230	On the importance of antiparallel C=O...C=O interactions in N1-(3-hydroxypropyl)-5-fluorouracilateHg(II) complex: A combined X-ray and DFT study. <i>Inorganica Chimica Acta</i> , 2016 , 452, 244-250	2.7	26
229	Synthesis and crystal structures of three new lead(II) isonicotinoylhydrazone derivatives: Anion controlled nuclearity and dimensionality. <i>Inorganica Chimica Acta</i> , 2017 , 461, 192-205	2.7	26
228	From monomers to polymers: steric and supramolecular effects on dimensionality of coordination architectures of heteroleptic mercury(II) halogenide-tetradentate Schiff base complexes. <i>CrystEngComm</i> , 2015 , 17, 3493-3502	3.3	26

227	Triple-bridged ferromagnetic nickel(II) complexes: a combined experimental and theoretical DFT study on stabilization and magnetic coupling. <i>Dalton Transactions</i> , 2014 , 43, 6455-67	4.3	26
226	A combined experimental and computational study of supramolecular assemblies in ternary copper(II) complexes with a tetradentate N4 donor Schiff base and halides. <i>RSC Advances</i> , 2014 , 4, 58643-58651	3.7	26
225	Surprising behaviour of MCO(lone pair)π(arene) interactions in the solid state of fluorinated oxaphosphirane complexes. <i>CrystEngComm</i> , 2015 , 17, 1769-1772	3.3	26
224	Competition between lone pair-πhalogen-πand triel bonding interactions involving BX3 (X = F, Cl, Br and I) compounds: an ab initio study. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	25
223	Concurrent aerogen bonding and lone pair/anion-πinteractions in the stability of organoxenon derivatives: a combined CSD and ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 30063-30068	3.6	25
222	Werner type clathrates involving guest benzoic acid and benzoate in discrete Mn(II) hosts: Experimental and theoretical studies. <i>Polyhedron</i> , 2019 , 159, 387-399	2.7	25
221	On the Versatility of BH X (X=F, Cl, Br, and I) Compounds as Halogen-, Hydrogen-, and Triel-Bond Donors: An Ab Initio Study. <i>ChemPhysChem</i> , 2016 , 17, 3181-3186	3.2	25
220	Role of ligand backbone of tridentate Schiff-base on complex nuclearity and bio-relevant catalytic activities of zinc(II) complexes: Experimental and theoretical investigations. <i>Inorganica Chimica Acta</i> , 2014 , 421, 364-373	2.7	25
219	Combined Experimental and Theoretical Investigation of Ligand and Anion Controlled Complex Formation with Unprecedented Structural Features and Photoluminescence Properties of Zinc(II) Complexes. <i>Crystal Growth and Design</i> , 2014 , 14, 4111-4123	3.5	25
218	Estimating ring strain energies in small carbocycles by means of the Bader's theory of Atoms-in-molecules. <i>Chemical Physics Letters</i> , 2012 , 536, 165-169	2.5	25
217	Importance of polarization assisted/resonance assisted hydrogen bonding interactions and unconventional interactions in crystal formations of five new complexes bearing chelidamic acid through a proton transfer mechanism. <i>RSC Advances</i> , 2015 , 5, 72923-72936	3.7	25
216	Cis-trans isomerism in diphenoxido bridged dicopper complexes: role of crystallized water to stabilize the cis isomer, variation in magnetic properties and conversion of both into a trinuclear species. <i>Dalton Transactions</i> , 2012 , 41, 12200-12	4.3	25
215	Synthesis, X-ray characterization, DFT calculations and Hirshfeld surface analysis of Zn(II) and Cd(II) complexes based on isonicotinoylhydrazone ligand. <i>CrystEngComm</i> , 2016 , 18, 4587-4596	3.3	25
214	Remote Control of Anion-πCatalysis on Fullerene-Centered Catalytic Triads. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 10883-10887	16.4	25
213	Supramolecular nanotubes based on halogen bonding interactions: cooperativity and interaction with small guests. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 12936-12941	3.6	24
212	Tetranuclear manganese(II) complexes of hydrazone and carbohydrazone ligands: Synthesis, crystal structures, magnetic properties, Hirshfeld surface analysis and DFT calculations. <i>Inorganica Chimica Acta</i> , 2016 , 443, 101-109	2.7	24
211	Experimental observation and theoretical investigation of a novel Cd(II) complex with πhole interactions involving nitro groups. <i>CrystEngComm</i> , 2015 , 17, 3912-3916	3.3	23
210	Ligand-Flexibility Controlled and Solvent-Induced Nuclearity Conversion in Cu(I)-Based Catecholase Models: A Deep Insight Through Combined Experimental and Theoretical Investigations. <i>European Journal of Inorganic Chemistry</i> , 2017 , 2017, 133-145	2.3	23

209	H-Bonded anion-anion complexes in fentanyl citrate polymorphs and solvates. <i>Chemical Communications</i> , 2019 , 55, 115-118	5.8	22
208	Hydrothermal synthesis, X-ray structure and DFT and magnetic studies of a (H ₂ SiW ₁₂ O ₄₀)(2-) based one-dimensional linear coordination polymer. <i>Dalton Transactions</i> , 2015 , 44, 8824-32	4.3	22
207	Formation of a water-mediated assembly of two neutral copper(II) Schiff base fragments with a Cu ₂ (NCS) ₄ moiety: exploration of non-covalent C-H...N (bimetallo ring) interactions. <i>CrystEngComm</i> , 2018 , 20, 1679-1689	3.3	22
206	Solvent-Triggered Cis/Trans Isomerism in Cobalt Dioxolene Chemistry: Distinguishing Effects of Packing on Valence Tautomerism. <i>Inorganic Chemistry</i> , 2016 , 55, 8331-40	5.1	22
205	Synthesis, X-ray characterization, DFT calculations and Hirshfeld surface analysis of thiosemicarbazone complexes of Mn ⁿ⁺ ions (n = 2, 3; M = Ni, Cd, Mn, Co and Cu). <i>CrystEngComm</i> , 2016 , 18, 1009-1023	3.3	22
204	Synthesis, crystal structure, magnetic property and DFT calculations of an unusual dinuclear μ-alkoxido bridged iron(III) complex. <i>Dalton Transactions</i> , 2013 , 42, 12274-83	4.3	22
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