Antonio Frontera

List of Publications by Year
in descending order

801 papers	27,203 citations	10650 74 h-index	19470 122 g-index
836 all docs	836 docs citations	836 times ranked	14161 citing authors

#	Article	IF	Citations
1	Anionâ€“Ï€ Interactions: Do They Exist?. Angewandte Chemie - International Edition, 2002, 41, 3389-3392.	7.2	690
2	OPLS all-atom force field for carbohydrates. Journal of Computational Chemistry, 1997, 18, 1955-1970.	1.5	619
3	Putting Anionâ€“Ï€ Interactions Into Perspective. Angewandte Chemie - International Edition, 2011, 50, 9564-9583.	7.2	591
4	Tetrelâ€Bonding Interaction: Rediscovered Supramolecular Force?. Angewandte Chemie - International Edition, 2013, 52, 12317-12321.	7.2	575
5	The Bright Future of Unconventional Ïƒ/Ï€â€Hole Interactions. ChemPhysChem, 2015, 16, 2496-2517.	1.0	569
6	Definition of the chalcogen bond (IUPAC Recommendations 2019). Pure and Applied Chemistry, 2019, 91, 1889-1892.	0.9	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.	1.4	304
8	Aerogen Bonding Interaction: A New Supramolecular Force?. Angewandte Chemie - International Edition, 2015, 54, 7340-7343.	7.2	294
9	Not Only Hydrogen Bonds: Other Noncovalent Interactions. Crystals, 2020, 10, 180.	1.0	289
10	Cooperativity in multiple unusual weak bonds. Theoretical Chemistry Accounts, 2010, 126, 1-14.	0.5	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.	2.3	243
12	Halogen bonding versuschalcogen and pnicogen bonding: a combined Cambridge structural database and theoretical study. CrystEngComm, 2013, 15, 3137-3144.	1.3	206
13	Anion Induced Formation of Supramolecular Associations Involving Lone pairâ‹¯Ï€ and Anionâ‹¯Ï€ Interactions in Co(II) Malonate Complexes: Experimental Observations, Hirshfeld Surface Analyses and DFT Studies. Inorganic Chemistry, 2012, 51, 3557-3571.	1.9	202
14	A Topological Analysis of the Electron Density in Anion-Ï€ Interactions. ChemPhysChem, 2003, 4, 1344-1348.	1.0	190
15	Tetrel Bonding Interactions. Chemical Record, 2016, 16, 473-487.	2.9	188
16	A thorough anionâ€“Ï€ interaction study in biomolecules: on the importance of cooperativity effects. Chemical Science, 2016, 7, 1038-1050.	3.7	188
17	Structure and Binding Energy of Anionâ‹¯Ï€ and Cationâ‹¯Ï€ Complexes:Â A Comparison of MP2, RI-MP2, DFT, and DF-DFT Methods. Journal of Physical Chemistry A, 2005, 109, 4632-4637.	1.1	186
18	Counterintuitive interaction of anions with benzene derivatives. Chemical Physics Letters, 2002, 359, 486-492.	1.2	178

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19	Anionâ€“Ï€ Interactions: Do They Exist?. Angewandte Chemie, 2002, 114, 3539-3542.	1.6	176
20	Cationâˆ’Ï€ versus Anionâˆ’Ï€ Interactions:Â Energetic, Charge Transfer, and Aromatic Aspects. Journal of Physical Chemistry A, 2004, 108, 9423-9427.	1.1	171
21	Anion-Ï€ Interactions in Cyanuric Acids: A Combined Crystallographic and Computational Study. Chemistry - A European Journal, 2005, 11, 6560-6567.	1.7	167
22	Relevant Anionâ€“Ï€ Interactions in Biological Systems: The Case of Urate Oxidase. Angewandte Chemie - International Edition, 2011, 50, 415-418.	7.2	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.	9.5	159
24	Cationâ€“Ï€ and anionâ€“Ï€ interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 440-459.	6.2	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.	1.4	151
26	Tetrel bonding interactions at work: Impact on tin and lead coordination compounds. Coordination Chemistry Reviews, 2019, 384, 107-125.	9.5	148
27	Interplay Between Cation-Ï€, Anion-Ï€ and Ï€-Ï€ Interactions. ChemPhysChem, 2006, 7, 2487-2491.	1.0	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.	9.5	140
29	Spodium Bonds: Noncovalent Interactions Involving Groupâ€…12 Elements. Angewandte Chemie - International Edition, 2020, 59, 17482-17487.	7.2	136
30	Directionality of Ï€-holes in nitro compounds. Chemical Communications, 2015, 51, 1491-1493.	2.2	130
31	1,2,4,5-Tetrazine: an unprecedented Î¼4-coordination that enhances ability for anionâ‹¯Ï€ interactions. Dalton Transactions, 2009, , 2856.	1.6	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.	1.6	124
33	Anionâ€“Ï€ interactions: must the aromatic ring be electron deficient?. New Journal of Chemistry, 2003, 27, 211-214.	1.4	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.	1.6	116
35	Pnicogenâ€“Ï€ complexes: theoretical study and biological implications. Physical Chemistry Chemical Physics, 2012, 14, 14061.	1.3	113
36	Encapsulation of anions: Macrocyclic receptors based on metal coordination and anionâ€“Ï€ interactions. Coordination Chemistry Reviews, 2013, 257, 1716-1727.	9.5	113

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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.	1.4	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.	1.6	106
39	Anionâˆ’Ï€ Interactions in Bisadenine Derivatives:â€‰ A Combined Crystallographic and Theoretical Study. Inorganic Chemistry, 2007, 46, 10724-10735.	1.9	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.	1.1	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	1.3	101
42	Towards design strategies for anionâ€“Ï€ interactions in crystal engineering. CrystEngComm, 2016, 18, 10-23.	1.3	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.	1.0	98
44	Ï€-Hole aerogen bonding interactions. Physical Chemistry Chemical Physics, 2015, 17, 24748-24753.	1.3	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.	1.4	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.	6.6	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.	6.6	96
48	s-Tetrazine as a new binding unit in molecular recognition of anions. Chemical Physics Letters, 2003, 370, 7-13.	1.2	95
49	Design of Lead(II) Metalâ€“Organic Frameworks Based on Covalent and Tetrel Bonding. Chemistry - A European Journal, 2015, 21, 17951-17958.	1.7	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.	2.2	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.	1.3	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.	1.1	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.	1.7	89
54	DABCO-Directed Self-Assembly of Bisporphyrins (DABCO=1,4-Diazabicyclo[2.2.2]octane). Chemistry - A European Journal, 2005, 11, 2196-2206.	1.7	88

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55	Supramolecular assemblies involving anionâ€“Ï€ and lone pairâ€“Ï€ interactions: experimental observation and theoretical analysis. CrystEngComm, 2011, 13, 4519.	1.3	86
56	Non-covalent sp³carbon bonding with ArCF₃is analogous to CHâ€“Ï€ interactions. Chemical Communications, 2014, 50, 12626-12629.	2.2	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.	1.0	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.	1.9	83
59	Ïƒ/Ï€-Hole noble gas bonding interactions: Insights from theory and experiment. Coordination Chemistry Reviews, 2020, 404, 213112.	9.5	83
60	Interplay between cation-Ï€ and hydrogen bonding interactions. Chemical Physics Letters, 2008, 456, 257-261.	1.2	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.	1.2	81
62	Regiumâ€“Ï€ bonds: An Unexplored Link between Noble Metal Nanoparticles and Aromatic Surfaces. Chemistry - A European Journal, 2018, 24, 7228-7234.	1.7	81
63	Quantification of Aromaticity in Oxocarbons: The Problem of the Fictitious â€œNonaromaticâ€•Reference System. Chemistry - A European Journal, 2002, 8, 433-438.	1.7	80
64	Very Longâ€Range Effects: Cooperativity between Anionâ€“Ï€ and Hydrogenâ€Bonding Interactions. ChemPhysChem, 2009, 10, 2256-2264.	1.0	80
65	Interplay between anionâ€Ï€ and hydrogen bonding interactions. Journal of Computational Chemistry, 2009, 30, 75-82.	1.5	79
66	Theoretical Study on Cooperativity Effects between Anionâ€“Ï€ and Halogenâ€Bonding Interactions. ChemPhysChem, 2011, 12, 2742-2750.	1.0	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.	1.9	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.	1.2	78
69	On the directionality of anionâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2011, 13, 5696.	1.3	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.	1.3	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.	1.6	78
72	Synergistic Anionâ€“(Ï€)_nâ€“Ï€ Catalysis on Ï€-Stacked Foldamers. Journal of the American Chemical Society, 2018, 140, 4884-4892.	6.6	78

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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.	1.6	78
74	A Strategy to Synthesize Molecular Knots and Links Using the Hydrophobic Effect. Journal of the American Chemical Society, 2018, 140, 12442-12450.	6.6	75
75	A theoretical study of aromaticity in squaramide and oxocarbons. Tetrahedron Letters, 2000, 41, 2001-2005.	0.7	74
76	Dual Binding Mode ofs-Triazine to Anions and Cations. Organic Letters, 2003, 5, 2227-2229.	2.4	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.	1.2	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.	1.2	74
79	Anionâ^'Ï€ Catalysis on Fullerenes. Journal of the American Chemical Society, 2017, 139, 13296-13299.	6.6	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.	1.6	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.	1.3	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.	1.9	73
83	Coordination Complexes Exhibiting AnionÂ·Â·Â·Ï€ Interactions: Synthesis, Structure, and Theoretical Studies. Inorganic Chemistry, 2008, 47, 5873-5881.	1.9	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.	1.9	72
85	NO3â^' anions can act as Lewis acid in the solid state. Nature Communications, 2017, 8, 14522.	5.8	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.	1.4	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.	1.1	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.	1.6	71
89	Importance of Râ€“CF₃Â·Â·Â·O Tetrel Bonding Interactions in Biological Systems. Journal of Physical Chemistry A, 2017, 121, 5371-5376.	1.1	69
90	RCH3Â·Â·Â·O Interactions in Biological Systems: Are They Trifurcated H-Bonds or Noncovalent Carbon Bonds?. Crystals, 2016, 6, 26.	1.0	68

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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.	1.0	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.	1.3	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.	1.9	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.	1.1	67
95	Ï€-Hole Interactions Involving Nitro Compounds: Directionality of Nitrate Esters. Crystal Growth and Design, 2016, 16, 5520-5524.	1.4	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.	1.7	66
97	A Cd(<scp>ii</scp>)-based MOF as a photosensitive Schottky diode: experimental and theoretical studies. Dalton Transactions, 2017, 46, 11239-11249.	1.6	66
98	Conformational Preferences and Self-Template Macrocyclization of Squaramide-Based Foldable Modules. Journal of Organic Chemistry, 2004, 69, 2302-2308.	1.7	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.	1.0	63
100	Ï€â€“hole interactions at work: crystal engineering with nitro-derivatives. CrystEngComm, 2017, 19, 1933-1937.	1.3	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.	1.3	63
102	Squaramide as a binding unit in molecular recognition. Chemical Physics Letters, 2000, 326, 247-254.	1.2	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.	0.5	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.	1.4	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.	0.9	62
106	Pnictogen-bonding catalysis: brevetoxin-type polyether cyclizations. Chemical Science, 2020, 11, 7086-7091.	3.7	62
107	Halogen and Chalcogen Bond Energies Evaluated Using Electron Density Properties. ChemPhysChem, 2020, 21, 26-31.	1.0	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.	1.6	61

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109	Experimental and theoretical study of uracil derivatives: the crucial role of weak fluorineâ€“fluorine noncovalent interactions. CrystEngComm, 2010, 12, 3758.	1.3	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.	1.6	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.	1.6	60
112	Anionâ‹…â‹…â‹…Anion Interactions Involving Ïƒâ€Holes of Perrhenate, Pertechnetate and Permanganate Anions. ChemPhysChem, 2021, 22, 2281-2285.	1.0	60
113	Molecular Electrostatic Potential and Noncovalent Interactions in Derivatives of Group 8 Elements. Angewandte Chemie - International Edition, 2021, 60, 20723-20727.	7.2	58
114	A theoretical study of aromaticity in squaramide complexes with anions. Chemical Physics Letters, 2002, 351, 115-120.	1.2	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.	1.3	57
116	Nature of Noncovalent Carbonâ€Bonding Interactions Derived from Experimental Chargeâ€Density Analysis. ChemPhysChem, 2015, 16, 2530-2533.	1.0	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.	1.3	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.	1.0	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.	1.6	56
120	Lithium diffusion in single-walled carbon nanotubes: a theoretical study. Chemical Physics Letters, 2003, 374, 548-555.	1.2	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.	1.3	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.	1.0	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.	3.7	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.	1.0	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.	1.6	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.	1.4	54

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127	Supramolecular Assembly of Metal Complexes by (Aryl)Iâ‹…â‹…â‹…d[Pt^{II}] Halogen Bonds. Chemistry - A European Journal, 2020, 26, 7692-7701.	1.7	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.	1.0	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.	1.4	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.	2.3	52
131	Energetic vs Synergetic Stability: A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 3266-3273.	1.1	52
132	Anionï¿Ï€ Interactions in Flavoproteins. Chemistry - an Asian Journal, 2011, 6, 2316-2318.	1.7	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.	1.2	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.	1.9	51
135	Ionpair-Ï€ interactions favor cell penetration of arginine/tryptophan-rich cell-penetrating peptides. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183098.	1.4	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.	1.7	50
137	MP2 Study of Cationâˆ'(Ï€)nâˆ'Ï€ Interactions (n= 1â€'4). Journal of Physical Chemistry A, 2006, 110, 9307-9309.	1.1	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.	1.2	49
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