David QuiÃ±onero

List of Publications by Year
in descending order

148 papers	7,788 citations	47 h-index	83 g-index
		47006	56724
157 all docs	157 docs citations	157 times ranked	5025 citing authors

#	Article	IF	Citations
1	Metastable Dianions and Dications. ChemPhysChem, 2020, 21, 1597-1607.	2.1	16
2	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
3	Hydrogen Bond versus Halogen Bond in HXOn (X = F, Cl, Br, and I) Complexes with Lewis Bases. Inorganics, 2019, 7, 9.	2.7	12
4	Unexpected chalcogen bonds in tetravalent sulfur compounds. Physical Chemistry Chemical Physics, 2019, 21, 11313-11319.	2.8	41
5	Cations brought together by hydrogen bonds: the protonated pyridineâ€“boronic acid dimer explained. Physical Chemistry Chemical Physics, 2019, 21, 5796-5802.	2.8	33
6	Hydrolysis of chemically distinct sites of human serum albumin by polyoxometalate: A hybrid QM/MM (ONIOM) study. Journal of Computational Chemistry, 2019, 40, 51-61.	3.3	17
7	Frontispiece: Adsorption and Quantification of Volatile Organic Compounds (VOCs) by using Hybrid Magnetic Nanoparticles. Chemistry - A European Journal, 2018, 24, .	3.3	0
8	Investigating Polyoxometalateâ€“Protein Interactions at Chemically Distinct Binding Sites. Journal of Physical Chemistry B, 2018, 122, 7219-7232.	2.6	27
9	Substituent Effects in Multivalent Halogen Bonding Complexes: A Combined Theoretical and Crystallographic Study. Molecules, 2018, 23, 18.	3.8	11
10	Adsorption and Quantification of Volatile Organic Compounds (VOCs) by using Hybrid Magnetic Nanoparticles. Chemistry - A European Journal, 2018, 24, 12820-12826.	3.3	14
11	Sigma-hole carbon-bonding interactions in carbonâ€“carbon double bonds: an unnoticed contact. Physical Chemistry Chemical Physics, 2017, 19, 15530-15540.	2.8	28
12	Hydrogen Bond versus Halogen Bond in Cationâ€“Cation Complexes: Effect of the Solvent. ChemPhysChem, 2017, 18, 3462-3468.	2.1	34
13	Weak interactions within nitryl halide heterodimers. New Journal of Chemistry, 2016, 40, 9060-9072.	2.8	8
14	Cationâ€“cation and anionâ€“anion complexes stabilized by halogen bonds. Physical Chemistry Chemical Physics, 2016, 18, 27939-27950.	2.8	45
15	A thorough anionâ€“Ï€ interaction study in biomolecules: on the importance of cooperativity effects. Chemical Science, 2016, 7, 1038-1050.	7.4	188
16	Anion Recognition by Pyrylium Cations and Thio-, Seleno- and Telluro- Analogues: A Combined Theoretical and Cambridge Structural Database Study. Molecules, 2015, 20, 11632-11659.	3.8	10
17	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
18	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

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19	Highly efficient coordination of Hg²⁺and Pb²⁺metals in water with squaramide-coated Fe₃O₄nanoparticles. Journal of Materials Chemistry A, 2014, 2, 8796-8803.	10.3	18
20	Thermodynamic Characterization of Halideâ˜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
21	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
22	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
23	Anionâ€“Ï€ interactions in [S4N3]+ rings. New Journal of Chemistry, 2013, 37, 2636.	2.8	17
24	Quadrupole moment versus Molecular Electrostatic Potential: Strange behavior of ethynyl-substituted benzenes. Chemical Physics Letters, 2013, 567, 60-65.	2.6	5
25	Halogen bonding versuschalcogen and pnicogen bonding: a combined Cambridge structural database and theoretical study. CrystEngComm, 2013, 15, 3137-3144.	2.6	206
26	Anionâ€“Ï€ Interactions Involving [MX_n]^{mâ^'} Anions: A Comprehensive Theoretical Study. ChemPhysChem, 2013, 14, 145-154.	2.1	11
27	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
28	Synthesis and structure ofcis-[RuCl(bpzm)(Îº¹-P-dpim)(Îº²-P,N-dpim)]ClÂ·(CHCl₃)₅. Stability of [Cl(HCCl₃)_n]^{â^'Â}aggregates. Supramolecular Chemistry, 2012, 24, 787-798.	1.2	1
29	Pnicogenâ€“Ï€ complexes: theoretical study and biological implications. Physical Chemistry Chemical Physics, 2012, 14, 14061.	2.8	113
30	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
31	Interplay between ionâ€“Ï€ and Ar/Ï€ Van der Waals interactions. Computational and Theoretical Chemistry, 2012, 998, 51-56.	2.5	12
32	Conformational Analysis of a Model Synthetic Prodiginine. Journal of Organic Chemistry, 2012, 77, 6538-6544.	3.2	15
33	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
34	Tuning of the anionâ€“Ï€ interaction. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	20
35	Theoretical ab initio study of anionâ€“Ï€ interactions in inorganic rings. Chemical Physics Letters, 2012, 530, 145-150.	2.6	17
36	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

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37	Unexpected Nonadditivity Effects in Anionâ^Ï€ Complexes. Journal of Physical Chemistry A, 2011, 115, 7849-7857.	2.5	23
38	RI-MP2 and MPWB1K Study of Ï€â€“Anionâ^Ï€â€² Complexes: MPWB1K Performance and Some Additivity Aspects. Journal of Chemical Theory and Computation, 2011, 7, 3012-3018.	5.3	26
39	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
40	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
41	On the directionality of anionâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2011, 13, 5696.	2.8	78
42	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
43	Self-assembly hexanuclear metallacontainer hosting halogenated guest species and sustaining structure of 3D coordination framework. Chemical Communications, 2011, 47, 1764-1766.	4.1	18
44	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
45	Anionï£¿Ï€ Interactions in Flavoproteins. Chemistry - an Asian Journal, 2011, 6, 2316-2318.	3.3	52
46	Can lone pair-Ï€ and cation-Ï€ interactions coexist? A theoretical study. Open Chemistry, 2011, 9, 25-34.	1.9	14
47	Cationâ€“Ï€ and anionâ€“Ï€ interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 440-459.	14.6	156
48	A methodological analysis for the assessment of non-covalent Ï€ interactions. Chemical Physics Letters, 2011, 508, 144-148.	2.6	23
49	Synthetic Tripodal SquaramidoâEBased Receptors for the Complexation of Antineoplastic Folates in Water. European Journal of Organic Chemistry, 2011, 2011, 6187-6194.	2.4	19
50	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
51	Theoretical Study on Cooperativity Effects between Anionâ€“Ï€ and HalogenâEBonding Interactions. ChemPhysChem, 2011, 12, 2742-2750.	2.1	79
52	Relevant Anionâ€“Ï€ Interactions in Biological Systems: The Case of Urate Oxidase. Angewandte Chemie - International Edition, 2011, 50, 415-418.	13.8	164
53	Synthetic Prodiginine Obatoclax (GX15â€070) and Related Analogues: Anion Binding, Transmembrane Transport, and Cytotoxicity Properties. Chemistry - A European Journal, 2011, 17, 14074-14083.	3.3	102
54	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

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55	Cooperativity in multiple unusual weak bonds. Theoretical Chemistry Accounts, 2010, 126, 1-14.	1.4	254
56	Cooperativity effects between non-covalent interactions: Are they important for Z-DNA stability?. Chemical Physics Letters, 2010, 485, 221-225.	2.6	13
57	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
58	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
59	A novel fluoride selective optical chemosensor based on internal charge transfer signaling. Tetrahedron Letters, 2010, 51, 596-599.	1.4	33
60	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
61	Experimental and theoretical study of uracil derivatives: the crucial role of weak fluorineâ€“fluorine noncovalent interactions. CrystEngComm, 2010, 12, 3758.	2.6	60
62	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
63	Experimental and computational study of the interplay between Câ€“H/Ï€ and anionâ€“Ï€ interactions. Dalton Transactions, 2010, 39, 794-806.	3.3	57
64	Computational Studies of the Geometry and Electronic Structure of an All-Inorganic and Homogeneous Tetra-Ru-Polyoxotungstate Catalyst for Water Oxidation and Its Four Subsequent One-Electron Oxidized Forms. Journal of Physical Chemistry A, 2010, 114, 535-542.	2.5	39
65	Substituent Effects in Ionâ‹¯Ï€ Interactions: Fine-Tuning via the Ethynyl Group. Journal of Physical Chemistry A, 2010, 114, 1926-1930.	2.5	22
66	New [2 Ã— 2] Copper(I) Grids as Anion Receptors. Effect of Ligand Functionalization on the Ability to Host Counteranions by Hydrogen Bonds. Inorganic Chemistry, 2010, 49, 8828-8847.	4.0	28
67	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
68	Very Longâ€Range Effects: Cooperativity between Anionâ€“Ï€ and Hydrogenâ€Bonding Interactions. ChemPhysChem, 2009, 10, 2256-2264.	2.1	80
69	Interplay between anionâ€Ï€ and hydrogen bonding interactions. Journal of Computational Chemistry, 2009, 30, 75-82.	3.3	79
70	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
71	Computational insights to the mechanism of alkene epoxidation by manganese-based catalysts in the presence of bicarbonate. Computational and Theoretical Chemistry, 2009, 903, 115-122.	1.5	13
72	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

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73	Interplay between cationâ€“Ï€ and hydrogen bonding interactions: Are non-additivity effects additive?. Chemical Physics Letters, 2009, 479, 316-320.	2.6	42
74	2-Aminopyrimidine Derivatives Exhibiting Anion-Ï€ Interactions: A Combined Crystallographic and Theoretical Study. Crystal Growth and Design, 2009, 9, 2363-2376.	3.0	39
75	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
76	Counterintuitive Substituent Effect of the Ethynyl Group in Ionâˆ’Ï€ Interactions. Journal of Physical Chemistry A, 2009, 113, 10367-10375.	2.5	43
77	Structural, Physicochemical, and Reactivity Properties of an All-Inorganic, Highly Active Tetraruthenium Homogeneous Catalyst for Water Oxidation. Journal of the American Chemical Society, 2009, 131, 17360-17370.	13.7	162
78	Energetic vs Synergetic Stability: A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 3266-3273.	2.5	52
79	Anionâˆ’Ï€ Interactions in Four-Membered Rings. Organic Letters, 2009, 11, 1987-1990.	4.6	38
80	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
81	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
82	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
83	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
84	Interplay between cation-Ï€ and hydrogen bonding interactions. Chemical Physics Letters, 2008, 456, 257-261.	2.6	82
85	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
86	Interplay between Edge-to-Face Aromatic and Hydrogen-Bonding Interactions. Journal of Physical Chemistry A, 2008, 112, 6017-6022.	2.5	24
87	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
88	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
89	Coordination Complexes Exhibiting AnionÂ·Â·Â·Ï€ Interactions: Synthesis, Structure, and Theoretical Studies. Inorganic Chemistry, 2008, 47, 5873-5881.	4.0	72
90	Molecular Interaction Potential with Polarization (MIPp) Study of the Interplay Between Ion-Ï€ and Hydrogen Bonding Interactions. The Open Chemical Physics Journal, 2008, 1, 36-41.	0.7	2

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91	Anionâˆ’Ï€ Interactions in Bisadenine Derivatives:â€‰ A Combined Crystallographic and Theoretical Study. Inorganic Chemistry, 2007, 46, 10724-10735.	4.0	104
92	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
93	MP2 study of cooperative effects between cationâ€“Ï€, anionâ€“Ï€ and Ï€âˆ’Ï€ interactions. New Journal of Chemistry, 2007, 31, 556-560.	2.8	151
94	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
95	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
96	A Theoretical Study of Anionâ€“Ï€ Interactions in Seven-Membered Rings. ChemPhysChem, 2007, 8, 1182-1187.	2.1	47
97	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
98	A density functional study of geometry and electronic structures of [(SiO4)(MIII)2(OH)2W10O32]4â^', M=Mo, Ru and Rh. Journal of Molecular Catalysis A, 2007, 262, 227-235.	4.8	10
99	The Role of the Central Atom in Structure and Reactivity of Polyoxometalates with Adjacent d-Electron Metal Sites. Computational and Experimental Studies of Î³-[(Xn+O4)RuIII2(OH)2(MFM)10O32](8-n)-for MFM= Mo and W, and X = AlIII, SiIV, PV, and SVI. Journal of Physical Chemistry B, 2006, 110, 170-173.	2.6	42
100	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
101	MP2 Study of Cationâ^'(Ï€)nâ^'Ï€ Interactions (n= 1â^'4). Journal of Physical Chemistry A, 2006, 110, 9307-9309.	2.5	49
102	Does Dinitrogen Hydrogenation Follow Different Mechanisms for [(Î·5-C5Me4H)2Zr]2(Î¼2,Î·2,Î·2-N2) and {[PhP(CH2SiMe2NSiMe2CH2)PPh]Zr}2(Î¼2,Î·2,Î·2-N2) Complexes? A Computational Study. Journal of the American Chemical Society, 2006, 128, 11391-11403.	13.7	35
103	Theoretical Study of the Structure and Properties of [(Î·5-C5Me4H)2Zr]2(Î¼2,Î·2,Î·2-N2). Journal of Chemical Theory and Computation, 2006, 2, 336-341.	5.3	6
104	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
105	A theoretical ab initio study of [n.n]paracyclophane complexes with cations. Chemical Physics Letters, 2006, 417, 371-377.	2.6	12
106	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
107	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
108	Interplay Between Cation-Ï€, Anion-Ï€ and Ï€-Ï€ Interactions. ChemPhysChem, 2006, 7, 2487-2491.	2.1	145

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109	A Squaramide-Based Citrate Receptor. Synfacts, 2006, 2006, 1225-1225.	0.0	0
110	Counterintuitive affinity of [2.2]paracyclophane to cations. Chemical Physics Letters, 2005, 408, 59-64.	2.6	14
111	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
112	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
113	Anion-Ï€ Interactions in Cyanuric Acids: A Combined Crystallographic and Computational Study. Chemistry - A European Journal, 2005, 11, 6560-6567.	3.3	167
114	Metalâˆ'Peroxo versus Metalâˆ'Oxo Oxidants in Non-Heme Iron-Catalyzed Olefin Oxidations:Â Computational and Experimental Studies on the Effect of Water. Journal of the American Chemical Society, 2005, 127, 6548-6549.	13.7	94
115	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
116	Preparation, Solid-State Characterization, and Computational Study of a Crown Ether Attached to a Squaramide. Organic Letters, 2005, 7, 1437-1440.	4.6	35
117	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
118	Anionâ€“Ï€ Interactions: Do They Exist?. Angewandte Chemie - International Edition, 2004, 43, 141-141.	13.8	3
119	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
120	Ab initio investigations of lithium diffusion in single-walled carbon nanotubes. Chemical Physics, 2004, 297, 85-91.	1.9	34
121	Structural and energetic features of single-walled carbon nanotube junctions: a theoretical ab initio study. Chemical Physics, 2004, 303, 265-270.	1.9	19
122	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
123	Cation-Ï€ vs anion-Ï€ interactions: a complete Ï€-orbital analysis. Chemical Physics Letters, 2004, 399, 220-225.	2.6	42
124	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
125	Anion-Ï€ interactions in five-membered rings: a combined crystallographic and ab initio study. Chemical Physics Letters, 2003, 382, 534-540.	2.6	41
126	A Topological Analysis of the Electron Density in Anion-Ï€ Interactions. ChemPhysChem, 2003, 4, 1344-1348.	2.1	190

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127	s-Tetrazine as a new binding unit in molecular recognition of anions. Chemical Physics Letters, 2003, 370, 7-13.	2.6	95
128	Lithium diffusion in single-walled carbon nanotubes: a theoretical study. Chemical Physics Letters, 2003, 374, 548-555.	2.6	55
129	Theoretical Studies of the Complex [(BPMEN)Fe(II)(NCCH3)2]2+, Precursor of Non-Heme Iron Catalysts for Olefin Epoxidation and Cis-Dihydroxylation. Inorganic Chemistry, 2003, 42, 8449-8455.	4.0	30
130	Dual Binding Mode ofs-Triazine to Anions and Cations. Organic Letters, 2003, 5, 2227-2229.	4.6	74
131	Weak Câ^'H/Ï€ Interaction Participates in the Diastereoselectivity of a Hostâ^'Guest Complex in the Presence of Six Strong Hydrogen Bonds. Organic Letters, 2003, 5, 1135-1138.	4.6	37
132	Anionâ€"Ï€ interactions: must the aromatic ring be electron deficient?. New Journal of Chemistry, 2003, 27, 211-214.	2.8	116
133	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
134	Anionâ€"Ï€ Interactions: Do They Exist?. Angewandte Chemie, 2002, 114, 3539-3542.	2.0	176
135	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
136	Anionâ€"Ï€ Interactions: Do They Exist?. Angewandte Chemie - International Edition, 2002, 41, 3389-3392.	13.8	690
137	Internal rotation in squaramide and related compounds. A theoretical ab initio study. Theoretical Chemistry Accounts, 2002, 108, 157-167.	1.4	2
138	A theoretical study of aromaticity in squaramide complexes with anions. Chemical Physics Letters, 2002, 351, 115-120.	2.6	57
139	Counterintuitive interaction of anions with benzene derivatives. Chemical Physics Letters, 2002, 359, 486-492.	2.6	178
140	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
141	Quantification of Aromaticity in Oxocarbons: The Problem of the Fictitious â€œNonaromaticâ€•Reference System. Chemistry - A European Journal, 2002, 8, 433.	3.3	0
142	OPLS all-atom force field for squaramides and squaric acid. Chemical Physics Letters, 2001, 350, 331-338.	2.6	12
143	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
144	The resonance model in amides: a combined crystallographic and ab initio investigation. New Journal of Chemistry, 2001, 25, 259-261.	2.8	15

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145	Squaramide as a binding unit in molecular recognition. Chemical Physics Letters, 2000, 326, 247-254.	2.6	62
146	A theoretical study of aromaticity in squaramide and oxocarbons. Tetrahedron Letters, 2000, 41, 2001-2005.	1.4	74
147	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
148	Squaramido-based receptors: applicability of molecular interaction potential to molecular recognition of polyalkylammonium compounds. Theoretical Chemistry Accounts, 2000, 104, 50-66.	1.4	9