

David Quiñónero

List of Publications by Year in descending order

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157
all docs

157
docs citations

157
times ranked

5025
citing authors

#	ARTICLE	IF	CITATIONS
1	Metastable Dianions and Dications. <i>ChemPhysChem</i> , 2020, 21, 1597-1607.	1.0	16
2	Influence of the aromatic surface on the capacity of adsorption of VOCs by magnetite supported organic-inorganic hybrids. <i>RSC Advances</i> , 2019, 9, 24184-24191.	1.7	10
3	Hydrogen Bond versus Halogen Bond in HXOn (X = F, Cl, Br, and I) Complexes with Lewis Bases. <i>Inorganics</i> , 2019, 7, 9.	1.2	12
4	Unexpected chalcogen bonds in tetravalent sulfur compounds. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11313-11319.	1.3	41
5	Cations brought together by hydrogen bonds: the protonated pyridine-boronic acid dimer explained. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5796-5802.	1.3	33
6	Hydrolysis of chemically distinct sites of human serum albumin by polyoxometalate: A hybrid QM/MM (ONIOM) study. <i>Journal of Computational Chemistry</i> , 2019, 40, 51-61.	1.5	17
7	Frontispiece: Adsorption and Quantification of Volatile Organic Compounds (VOCs) by using Hybrid Magnetic Nanoparticles. <i>Chemistry - A European Journal</i> , 2018, 24, .	1.7	0
8	Investigating Polyoxometalate-Protein Interactions at Chemically Distinct Binding Sites. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7219-7232.	1.2	27
9	Substituent Effects in Multivalent Halogen Bonding Complexes: A Combined Theoretical and Crystallographic Study. <i>Molecules</i> , 2018, 23, 18.	1.7	11
10	Adsorption and Quantification of Volatile Organic Compounds (VOCs) by using Hybrid Magnetic Nanoparticles. <i>Chemistry - A European Journal</i> , 2018, 24, 12820-12826.	1.7	14
11	Sigma-hole carbon-bonding interactions in carbon-carbon double bonds: an unnoticed contact. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15530-15540.	1.3	28
12	Hydrogen Bond versus Halogen Bond in Cation-Cation Complexes: Effect of the Solvent. <i>ChemPhysChem</i> , 2017, 18, 3462-3468.	1.0	34
13	Weak interactions within nitril halide heterodimers. <i>New Journal of Chemistry</i> , 2016, 40, 9060-9072.	1.4	8
14	Cation-cation and anion-anion complexes stabilized by halogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27939-27950.	1.3	45
15	A thorough anion- π interaction study in biomolecules: on the importance of cooperativity effects. <i>Chemical Science</i> , 2016, 7, 1038-1050.	3.7	188
16	Anion Recognition by Pyrylium Cations and Thio-, Seleno- and Telluro- Analogues: A Combined Theoretical and Cambridge Structural Database Study. <i>Molecules</i> , 2015, 20, 11632-11659.	1.7	10
17	Reconciling Experiment and Theory in the Use of Aryl-Extended Calix[4]pyrrole Receptors for the Experimental Quantification of Chloride- π Interactions in Solution. <i>International Journal of Molecular Sciences</i> , 2015, 16, 8934-8948.	1.8	10
18	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, 1322-1326.	1.3	28

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19	Highly efficient coordination of Hg ²⁺ and Pb ²⁺ metals in water with squaramide-coated Fe ₃ O ₄ nanoparticles. <i>Journal of Materials Chemistry A</i> , 2014, 2, 8796-8803.	5.2	18
20	Thermodynamic Characterization of Halide ⁻ Interactions in Solution Using α -Two-Wall α -Aryl Extended Calix[4]pyrroles as Model System. <i>Journal of the American Chemical Society</i> , 2014, 136, 3208-3218.	6.6	96
21	Long-Range Effects in Anion ⁻ Interactions: Their Crucial Role in the Inhibition Mechanism of <i>Mycobacterium Tuberculosis</i> Malate Synthase. <i>Chemistry - A European Journal</i> , 2014, 20, 6985-6990.	1.7	35
22	On the Importance of Anion ⁻ Interactions in the Mechanism of Sulfide:Quinone Oxidoreductase. <i>Chemistry - an Asian Journal</i> , 2013, 8, 2708-2713.	1.7	31
23	Anion ⁻ interactions in [S ₄ N ₃] ⁺ rings. <i>New Journal of Chemistry</i> , 2013, 37, 2636.	1.4	17
24	Quadrupole moment versus Molecular Electrostatic Potential: Strange behavior of ethynyl-substituted benzenes. <i>Chemical Physics Letters</i> , 2013, 567, 60-65.	1.2	5
25	Halogen bonding versus chalcogen and pnictogen bonding: a combined Cambridge structural database and theoretical study. <i>CrystEngComm</i> , 2013, 15, 3137-3144.	1.3	206
26	Anion ⁻ Interactions Involving [MX _n] ^{m+} Anions: A Comprehensive Theoretical Study. <i>ChemPhysChem</i> , 2013, 14, 145-154.	1.0	11
27	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, 2651-2655.	1.1	38
28	Synthesis and structure of <i>cis</i> -[RuCl(bpzm)(¹ P)(² P,N)-dpim]Cl \cdot (CHCl ₃) ₅ . Stability of [Cl(HCCl ₃) _n] ⁿ⁺ aggregates. <i>Supramolecular Chemistry</i> , 2012, 24, 787-798.	1.5	1
29	Pnictogen ⁻ complexes: theoretical study and biological implications. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14061.	1.3	113
30	Theoretical ab initio study of lone pair and anion ⁻ interactions in fluorinated tropolones. <i>Computational and Theoretical Chemistry</i> , 2012, 998, 20-25.	1.1	7
31	Interplay between ion ⁻ and Ar ⁻ Van der Waals interactions. <i>Computational and Theoretical Chemistry</i> , 2012, 998, 51-56.	1.1	12
32	Conformational Analysis of a Model Synthetic Prodiginine. <i>Journal of Organic Chemistry</i> , 2012, 77, 6538-6544.	1.7	15
33	Feasibility of Single-Walled Carbon Nanotubes as Materials for CO ₂ Adsorption: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 21083-21092.	1.5	32
34	Tuning of the anion ⁻ interaction. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	20
35	Theoretical ab initio study of anion ⁻ interactions in inorganic rings. <i>Chemical Physics Letters</i> , 2012, 530, 145-150.	1.2	17
36	Estimating ring strain energies in small carbocycles by means of the Bader TM s theory of $\tilde{\text{atoms-in-molecules}}^{\text{TM}}$. <i>Chemical Physics Letters</i> , 2012, 536, 165-169.	1.2	27

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37	Unexpected Nonadditivity Effects in Anion-π Complexes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7849-7857.	1.1	23
38	RI-MP2 and MPWB1K Study of π-π Anion-π ² Complexes: MPWB1K Performance and Some Additivity Aspects. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3012-3018.	2.3	26
39	Kinetics and mechanism of the oxidation of hydroxylamine by a {Mn3O4}4+ core in aqueous acidic media. <i>Dalton Transactions</i> , 2011, 40, 9571.	1.6	2
40	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.	1.3	92
41	On the directionality of anion-π interactions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5696.	1.3	78
42	Radical cation (C ^{•+}) and radical anion (A ^{•-}) interactions with aromatic rings: energetic, orbitalic and spin density considerations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16698.	1.3	13
43	Self-assembly hexanuclear metallacontainer hosting halogenated guest species and sustaining structure of 3D coordination framework. <i>Chemical Communications</i> , 2011, 47, 1764-1766.	2.2	18
44	Theoretical ab initio study of substituted benzene trimer: Interplay between hydrogen bonding and π-π interactions. <i>Computational and Theoretical Chemistry</i> , 2011, 975, 106-110.	1.1	7
45	Anion-π Interactions in Flavoproteins. <i>Chemistry - an Asian Journal</i> , 2011, 6, 2316-2318.	1.7	52
46	Can lone pair-π and cation-π interactions coexist? A theoretical study. <i>Open Chemistry</i> , 2011, 9, 25-34.	1.0	14
47	Cation-π and anion-π interactions. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 440-459.	6.2	156
48	A methodological analysis for the assessment of non-covalent π interactions. <i>Chemical Physics Letters</i> , 2011, 508, 144-148.	1.2	23
49	Synthetic Tripodal Squaramido-Based Receptors for the Complexation of Antineoplastic Folates in Water. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 6187-6194.	1.2	19
50	The Role of the Ethynyl Substituent on the π-π Stacking Affinity of Benzene: A Theoretical Study. <i>ChemPhysChem</i> , 2011, 12, 283-288.	1.0	3
51	Theoretical Study on Cooperativity Effects between Anion-π and Halogen-Bonding Interactions. <i>ChemPhysChem</i> , 2011, 12, 2742-2750.	1.0	79
52	Relevant Anion-π Interactions in Biological Systems: The Case of Urate Oxidase. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 415-418.	7.2	164
53	Synthetic Prodiginine Obatoclox (GX15070) and Related Analogues: Anion Binding, Transmembrane Transport, and Cytotoxicity Properties. <i>Chemistry - A European Journal</i> , 2011, 17, 14074-14083.	1.7	102
54	Anion-π, lone pair-π, and F...F interactions in nucleobase derivatives. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2011, 67, C600-C601.	0.3	0

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55	Cooperativity in multiple unusual weak bonds. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 1-14.	0.5	254
56	Cooperativity effects between non-covalent interactions: Are they important for Z-DNA stability?. <i>Chemical Physics Letters</i> , 2010, 485, 221-225.	1.2	13
57	New Chlorido(dimethyl sulfoxide)iridium(III) Complexes with N6-Substituted Adenines - Kinetic N(7) versus Thermodynamic N(9) Coordinated Adenine Isomers. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 5617-5628.	1.0	10
58	A Combined Experimental and Theoretical Study of Anion \cdots Interactions in $N_{6,9}$ - and $N_{7,9}$ -Decyladenine Salts. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 5171-5180.	1.2	19
59	A novel fluoride selective optical chemosensor based on internal charge transfer signaling. <i>Tetrahedron Letters</i> , 2010, 51, 596-599.	0.7	33
60	Erroneous behaviour of the widely used MP2(full)/aug-cc-pVXZ (X=D,T) level of theory for evaluating the BSSE in ion \cdots complexes. <i>Chemical Physics Letters</i> , 2010, 489, 254-258.	1.2	20
61	Experimental and theoretical study of uracil derivatives: the crucial role of weak fluorine \cdots fluorine noncovalent interactions. <i>CrystEngComm</i> , 2010, 12, 3758.	1.3	60
62	New 1,8-naphthyridine-based probes for the selective fluorescence signalling of toxic cadmium: synthesis, photophysical studies and molecular modelling. <i>Supramolecular Chemistry</i> , 2010, 22, 524-531.	1.5	4
63	Experimental and computational study of the interplay between C \cdots H/ \cdots and anion \cdots interactions. <i>Dalton Transactions</i> , 2010, 39, 794-806.	1.6	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. <i>Journal of Physical Chemistry A</i> , 2010, 114, 535-542.	1.1	39
65	Substituent Effects in Ion \cdots Interactions: Fine-Tuning via the Ethynyl Group. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1926-1930.	1.1	22
66	New [2 \times 2] Copper(I) Grids as Anion Receptors. Effect of Ligand Functionalization on the Ability to Host Counteranions by Hydrogen Bonds. <i>Inorganic Chemistry</i> , 2010, 49, 8828-8847.	1.9	28
67	Lone pair \cdots vs $\pi\cdots\pi$ interactions in 5-fluoro-1-hexyluracil and 1-hexyluracil: a combined crystallographic and computational study. <i>CrystEngComm</i> , 2010, 12, 362-365.	1.3	39
68	Very Long-Range Effects: Cooperativity between Anion \cdots and Hydrogen \cdots Bonding Interactions. <i>ChemPhysChem</i> , 2009, 10, 2256-2264.	1.0	80
69	Interplay between anion \cdots and hydrogen bonding interactions. <i>Journal of Computational Chemistry</i> , 2009, 30, 75-82.	1.5	79
70	Theoretical ab initio study of the interplay between hydrogen bonding, cation \cdots and $\pi\cdots\pi$ interactions. <i>Theoretical Chemistry Accounts</i> , 2009, 122, 325-332.	0.5	31
71	Computational insights to the mechanism of alkene epoxidation by manganese-based catalysts in the presence of bicarbonate. <i>Computational and Theoretical Chemistry</i> , 2009, 903, 115-122.	1.5	13
72	Theoretical and crystallographic study of edge-to-face aromatic interactions between pyridine moieties and benzene. <i>Chemical Physics Letters</i> , 2009, 468, 280-285.	1.2	21

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73	Interplay between cation- π and hydrogen bonding interactions: Are non-additivity effects additive?. <i>Chemical Physics Letters</i> , 2009, 479, 316-320.	1.2	42
74	2-Aminopyrimidine Derivatives Exhibiting Anion- π Interactions: A Combined Crystallographic and Theoretical Study. <i>Crystal Growth and Design</i> , 2009, 9, 2363-2376.	1.4	39
75	Simultaneous Interaction of Tetrafluoroethene with Anions and Hydrogen-Bond Donors: A Cooperativity Study. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1186-1194.	2.3	52
76	Counterintuitive Substituent Effect of the Ethynyl Group in Ion- π Interactions. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10367-10375.	1.1	43
77	Structural, Physicochemical, and Reactivity Properties of an All-Inorganic, Highly Active Tetraruthenium Homogeneous Catalyst for Water Oxidation. <i>Journal of the American Chemical Society</i> , 2009, 131, 17360-17370.	6.6	162
78	Energetic vs Synergetic Stability: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3266-3273.	1.1	52
79	Anion- π Interactions in Four-Membered Rings. <i>Organic Letters</i> , 2009, 11, 1987-1990.	2.4	38
80	MP2 Study of synergistic effects between X-H ($X = C, N, O$) and π - π interactions. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 385-393.	0.5	62
81	High-Level Ab Initio Study of Anion- π Interactions in Pyridine and Pyrazine Rings Coordinated to Ag ^I . <i>ChemPhysChem</i> , 2008, 9, 397-399.	1.0	53
82	Crystallographic and Theoretical Evidence of Anion- π and Hydrogen-Bonding Interactions in a Squaramide-Nitrate Salt. <i>European Journal of Organic Chemistry</i> , 2008, 2008, 1864-1868.	1.2	49
83	On the importance of the inclusion of the basis set superposition error counterpoise correction during optimization of ion- π complexes. <i>Chemical Physics Letters</i> , 2008, 455, 325-330.	1.2	13
84	Interplay between cation- π and hydrogen bonding interactions. <i>Chemical Physics Letters</i> , 2008, 456, 257-261.	1.2	82
85	Interaction of positively and negatively charged aromatic hydrocarbons with benzene and triphenylene: Towards a model of pure organic insulators. <i>Chemical Physics Letters</i> , 2008, 460, 406-410.	1.2	36
86	Interplay between Edge-to-Face Aromatic and Hydrogen-Bonding Interactions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6017-6022.	1.1	24
87	MP2 Study of the Dual π - π Anion-Binding Affinity of Fluorinated Phthalic Acid Anhydrides. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1622-1626.	1.1	12
88	Theoretical and Crystallographic Study of the Dual π - π Anion Binding Affinity of Quinolizinylium Cation. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1981-1989.	2.3	21
89	Coordination Complexes Exhibiting Anion- π Interactions: Synthesis, Structure, and Theoretical Studies. <i>Inorganic Chemistry</i> , 2008, 47, 5873-5881.	1.9	72
90	Molecular Interaction Potential with Polarization (MIPp) Study of the Interplay Between Ion- π and Hydrogen Bonding Interactions. <i>The Open Chemical Physics Journal</i> , 2008, 1, 36-41.	0.7	2

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91	Anion-π Interactions in Bisadenine Derivatives: A Combined Crystallographic and Theoretical Study. <i>Inorganic Chemistry</i> , 2007, 46, 10724-10735.	1.9	104
92	Dual Cation and Anion Acceptor Molecules. The Case of the (1-6-C6H6)(1-6C6F6)Cr(0) Complex. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3137-3142.	1.1	29
93	MP2 study of cooperative effects between cation-π, anion-π and π-π interactions. <i>New Journal of Chemistry</i> , 2007, 31, 556-560.	1.4	151
94	Induced-Polarization Energy Map: A Helpful Tool for Predicting Geometric Features of Anion-π Complexes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2098-2107.	2.3	20
95	A Combined Experimental and Theoretical Study of Anion-π Interactions in Bis(pyr-imidine) Salts. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 5821-5825.	1.2	29
96	A Theoretical Study of Anion-π Interactions in Seven-Membered Rings. <i>ChemPhysChem</i> , 2007, 8, 1182-1187.	1.0	47
97	MP2 study of anion-π complexes of trifluoro-s-triazine with tetrahedral and octahedral anions. <i>Chemical Physics Letters</i> , 2007, 438, 104-108.	1.2	29
98	A density functional study of geometry and electronic structures of [(SiO4)(MIII)2(OH)2W10O32]4-, M=Mo, Ru and Rh. <i>Journal of Molecular Catalysis A</i> , 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 3-[(Xn+O4)RuIII2(OH)2(MFM)10O32](8-n)-for MFM= Mo and W, and X = AlIII, SiIV, PV, and SVI. <i>Journal of Physical Chemistry B</i> , 2006, 110, 170-173.	1.2	42
100	Ab Initio Study of [n.n]Paracyclophane (n= 2, 3) Complexes with Cations: An Unprecedented Through-Space Substituent Effects. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5144-5148.	1.1	71
101	MP2 Study of Cation-π Interactions (n= 1-4). <i>Journal of Physical Chemistry A</i> , 2006, 110, 9307-9309.	1.1	49
102	Does Dinitrogen Hydrogenation Follow Different Mechanisms for [(1-5-C5Me4H)2Zr]2(1/2,1/2,1/2-N2) and [(PhP(CH2SiMe2NSiMe2CH2)PPh)Zr]2(1/2,1/2,1/2-N2) Complexes? A Computational Study. <i>Journal of the American Chemical Society</i> , 2006, 128, 11391-11403.	6.6	35
103	Theoretical Study of the Structure and Properties of [(1-5-C5Me4H)2Zr]2(1/2,1/2,1/2-N2). <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 336-341.	2.3	6
104	Rational Design, Synthesis, and Application of a New Receptor for the Molecular Recognition of Tricarboxylate Salts in Aqueous Media. <i>Journal of Organic Chemistry</i> , 2006, 71, 7185-7195.	1.7	66
105	A theoretical ab initio study of [n.n]paracyclophane complexes with cations. <i>Chemical Physics Letters</i> , 2006, 417, 371-377.	1.2	12
106	Synthesis, X-ray structure analysis and computational studies of novel bis(thiocarbamoyl) disulfides with non-covalent S-N and S-S interactions. <i>Chemical Physics Letters</i> , 2006, 422, 234-239.	1.2	24
107	Affinity of ferrocene and (1,1-ε²)(3,3-ε²)[3,3]ferrocenophane to cations. <i>Chemical Physics Letters</i> , 2006, 424, 204-208.	1.2	4
108	Interplay Between Cation-π, Anion-π and π-π Interactions. <i>ChemPhysChem</i> , 2006, 7, 2487-2491.	1.0	145

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109	A Squaramide-Based Citrate Receptor. <i>Synfacts</i> , 2006, 2006, 1225-1225.	0.0	0
110	Counterintuitive affinity of [2.2]paracyclophane to cations. <i>Chemical Physics Letters</i> , 2005, 408, 59-64.	1.2	14
111	Ab initio investigations of lithium insertion in boron and nitrogen-doped single-walled carbon nanotubes. <i>Chemical Physics Letters</i> , 2005, 411, 256-261.	1.2	24
112	A Theoretical ab initio Study of the Capacity of Several Binding Units for the Molecular Recognition of Anions. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 179-183.	1.2	74
113	Anion- π Interactions in Cyanuric Acids: A Combined Crystallographic and Computational Study. <i>Chemistry - A European Journal</i> , 2005, 11, 6560-6567.	1.7	167
114	Metal π -Peroxo versus Metal π -Oxo Oxidants in Non-Heme Iron-Catalyzed Olefin Oxidations: A Computational and Experimental Studies on the Effect of Water. <i>Journal of the American Chemical Society</i> , 2005, 127, 6548-6549.	6.6	94
115	Approximate Additivity of Anion π Interactions: An Ab Initio Study on Anion π , Anion π_2 and Anion π_3 Complexes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9341-9345.	1.1	101
116	Preparation, Solid-State Characterization, and Computational Study of a Crown Ether Attached to a Squaramide. <i>Organic Letters</i> , 2005, 7, 1437-1440.	2.4	35
117	Structure and Binding Energy of Anion π and Cation π Complexes: A Comparison of MP2, RI-MP2, DFT, and DF-DFT Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4632-4637.	1.1	186
118	Anion π Interactions: Do They Exist?. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 141-141.	7.2	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. <i>Tetrahedron Letters</i> , 2004, 45, 9387-9391.	0.7	8
120	Ab initio investigations of lithium diffusion in single-walled carbon nanotubes. <i>Chemical Physics</i> , 2004, 297, 85-91.	0.9	34
121	Structural and energetic features of single-walled carbon nanotube junctions: a theoretical ab initio study. <i>Chemical Physics</i> , 2004, 303, 265-270.	0.9	19
122	Cation π versus anion π interactions: a comparative ab initio study based on energetic, electron charge density and aromatic features. <i>Chemical Physics Letters</i> , 2004, 392, 85-89.	1.2	74
123	Cation π vs anion π interactions: a complete π -orbital analysis. <i>Chemical Physics Letters</i> , 2004, 399, 220-225.	1.2	42
124	Cation π versus Anion π Interactions: Energetic, Charge Transfer, and Aromatic Aspects. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9423-9427.	1.1	171
125	Anion π interactions in five-membered rings: a combined crystallographic and ab initio study. <i>Chemical Physics Letters</i> , 2003, 382, 534-540.	1.2	41
126	A Topological Analysis of the Electron Density in Anion π Interactions. <i>ChemPhysChem</i> , 2003, 4, 1344-1348.	1.0	190

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127	s-Tetrazine as a new binding unit in molecular recognition of anions. <i>Chemical Physics Letters</i> , 2003, 370, 7-13.	1.2	95
128	Lithium diffusion in single-walled carbon nanotubes: a theoretical study. <i>Chemical Physics Letters</i> , 2003, 374, 548-555.	1.2	55
129	Theoretical Studies of the Complex [(BPMEN)Fe(II)(NCCH ₃) ₂] ²⁺ , Precursor of Non-Heme Iron Catalysts for Olefin Epoxidation and Cis-Dihydroxylation. <i>Inorganic Chemistry</i> , 2003, 42, 8449-8455.	1.9	30
130	Dual Binding Mode of s-Triazine to Anions and Cations. <i>Organic Letters</i> , 2003, 5, 2227-2229.	2.4	74
131	Weak C-H...N Interaction Participates in the Diastereoselectivity of a Host-Guest Complex in the Presence of Six Strong Hydrogen Bonds. <i>Organic Letters</i> , 2003, 5, 1135-1138.	2.4	37
132	Anion-π interactions: must the aromatic ring be electron deficient?. <i>New Journal of Chemistry</i> , 2003, 27, 211-214.	1.4	116
133	Predicting Experimental Complexation-Induced Changes in ¹ H NMR Chemical Shift for Complexes between Zinc-Porphyrins and Amines Using the ab Initio/GIAO-HF Methodology. <i>Organic Letters</i> , 2002, 4, 399-401.	2.4	30
134	Anion-π Interactions: Do They Exist?. <i>Angewandte Chemie</i> , 2002, 114, 3539-3542.	1.6	176
135	Quantification of Aromaticity in Oxocarbons: The Problem of the Fictitious "Nonaromatic" Reference System. <i>Chemistry - A European Journal</i> , 2002, 8, 433-438.	1.7	80
136	Anion-π Interactions: Do They Exist?. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 3389-3392.	7.2	690
137	Internal rotation in squaramide and related compounds. A theoretical ab initio study. <i>Theoretical Chemistry Accounts</i> , 2002, 108, 157-167.	0.5	2
138	A theoretical study of aromaticity in squaramide complexes with anions. <i>Chemical Physics Letters</i> , 2002, 351, 115-120.	1.2	57
139	Counterintuitive interaction of anions with benzene derivatives. <i>Chemical Physics Letters</i> , 2002, 359, 486-492.	1.2	178
140	Predicting experimental complexation-induced changes in NMR chemical shift for complexes between metalloporphyrins and ligands using the Ab initio/GIAO-HF methodology. <i>Chemical Physics Letters</i> , 2002, 360, 72-78.	1.2	6
141	OPLS all-atom force field for squaramides and squaric acid. <i>Chemical Physics Letters</i> , 2001, 350, 331-338.	1.2	12
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145	A theoretical study of aromaticity in squaramide and oxocarbons. <i>Tetrahedron Letters</i> , 2000, 41, 2001-2005.	0.7	74
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