Jordi Poater

List of Publications by Year in descending order

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156 papers	8,287 citations	47 h-index	86 g-index
		47006	51608
165 all docs	165 docs citations	165 times ranked	5324 citing authors

#	Article	IF	Citations
1	Path-dependency of energy decomposition analysis & the elusive nature of bonding. Physical Chemistry Chemical Physics, 2022, 24, 2344-2348.	2.8	27
2	C(spⁿ)â^'X (n=1â€“3) Bond Activation by Palladium. Chemistry - A European Journal, 2022, 28, .	3.3	7
3	Probing the Lewis Acidity of Boronic Acids through Interactions with Arene Substituents. Chemistry - A European Journal, 2022, 28, .	3.3	8
4	Rational design of iron catalysts for C â€“ X bond activation. Journal of Computational Chemistry, 2022, , .	3.3	7
5	Aromaticity and Extrusion of Benzenoids Linked to [oâ€COSAN]^{â^'}: Clar Has the Answer. Angewandte Chemie - International Edition, 2022, 61, .	13.8	12
6	Reading and erasing of the phosphonium analogue of trimethyllysine by epigenetic proteins. Communications Chemistry, 2022, 5, .	4.5	5
7	Câ^'X Bond Activation by Palladium: Steric Shielding versus Steric Attraction. Chemistry - A European Journal, 2022, 28, .	3.3	11
8	Probing Noncovalent Interactions in [3,3]Metaparacyclophanes. Journal of Organic Chemistry, 2022, 87, 6087-6096.	3.2	2
9	Through-Space Stabilization of an Imidazolium Cation by Aromatic Rings. Journal of Organic Chemistry, 2022, 87, 7875-7883.	3.2	2
10	3D and 2D aromatic units behave like oil and water in the case of benzocarborane derivatives. Nature Communications, 2022, 13, .	12.8	23
11	Bismutamide als einfache Vermittler hochselektiver Pnâ^'Pnâ€Radikalâ€Kupplungsreaktionen (Pn=N, P, As). Angewandte Chemie, 2021, 133, 6513-6518.	2.0	7
12	Bismuth Amides Mediate Facile and Highly Selective Pnâ€“Pn Radicalâ€Coupling Reactions (Pn=N, P, As). Angewandte Chemie - International Edition, 2021, 60, 6441-6445.	13.8	36
13	The energy components of the extended transition state energy decomposition analysis are path functions: the case of water tetramer. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	8
14	Do Sulfonamides Interact with Aromatic Rings?. Chemistry - A European Journal, 2021, 27, 5721-5729.	3.3	7
15	Chelation enforcing a dual gold configuration in the catalytic hydroxyphenoxylation of alkynes. Applied Organometallic Chemistry, 2021, 35, e6362.	3.5	5
16	Pyrrole and Pyridine in the Water Environmentâ€"Effect of Discrete and Continuum Solvation Models. ACS Omega, 2021, 6, 24693-24699.	3.5	4
17	Cage^{â€“}Â·Â·Â·Cage^{â€“} Interaction: Boron Cluster-Based Noncovalent Bond and Its Applications in Solid-State Materials. Jacs Au, 2021, 1, 2047-2057.	7.9	5
18	The Chemical Bond: When Atom Size Instead of Electronegativity Difference Determines Trend in Bond Strength. Chemistry - A European Journal, 2021, 27, 15616-15622.	3.3	26

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19	Zwitterionic Aromaticity on Azulene Extrapolated to carboâ€Azulene. European Journal of Organic Chemistry, 2021, 2021, 6450-6458.	2.4	5
20	Phenoxylation of Alkynes through Monoâ€•and Dual Activation Using Group 11 (Cu, Ag, Au) Catalysts. European Journal of Inorganic Chemistry, 2020, 2020, 1123-1134.	2.0	7
21	Activation Strain Analyses of Counterion and Solvent Effects on the Ionâ€Pair S N 2 Reaction of and CH 3 Cl. Journal of Computational Chemistry, 2020, 41, 317-327.	3.3	4
22	Distortionâ€Controlled Redshift of Organic Dye Molecules. Chemistry - A European Journal, 2020, 26, 2080-2093.	3.3	12
23	Probing Halogenâˆ™Ï€ versus CHâˆ™Ï€ Interactions in Molecular Balance. Organic Letters, 2020, 22, 7870-7873.	4.6	11
24	Analysis of the electronic delocalization in some isoelectronic analogues of B₁₂ doped with beryllium and/or carbon. Physical Chemistry Chemical Physics, 2020, 22, 12245-12259.	2.8	12
25	Cyclopropenylidenephosphoranes: Rearrangement to Azetidinylidene-Methylphosphoniums. Journal of Organic Chemistry, 2020, 85, 7452-7458.	3.2	2
26	Mechanism of biomolecular recognition of trimethyllysine by the fluorinated aromatic cage of KDM5A PHD3 finger. Communications Chemistry, 2020, 3, .	4.5	13
27	Throughâ€Space Polarâ€Ï€ Interactions in 2,6â€Diarylthiophenols. ChemPhysChem, 2020, 21, 1080-1080.	2.1	0
28	The nido â€Cageâ‹…â‹…â‹…Ï€ Bond: A Nonâ€covalent Interaction between Boron Clusters and Aromatic Rings and Its Applications. Angewandte Chemie, 2020, 132, 9103-9110.	2.0	7
29	The nidoâ€Cageâ‹…â‹…â‹…Ï€ Bond: A Nonâ€covalent Interaction between Boron Clusters and Aromatic Rings and Its Applications. Angewandte Chemie - International Edition, 2020, 59, 9018-9025.	13.8	32
30	Throughâ€Space Polarâ€Ï€ Interactions in 2,6â€Diarylthiophenols. ChemPhysChem, 2020, 21, 1092-1100.	2.1	9
31	Comparison of Molecular Recognition of Trimethyllysine and Trimethylthialysine by Epigenetic Reader Proteins. Molecules, 2020, 25, 1918.	3.8	8
32	Too Persistent to Give Up: Aromaticity in Boron Clusters Survives Radical Structural Changes. Journal of the American Chemical Society, 2020, 142, 9396-9407.	13.7	145
33	PyFrag 2019â€”Automating the exploration and analysis of reaction mechanisms. Journal of Computational Chemistry, 2019, 40, 2227-2233.	3.3	57
34	Carbon monoxide insertion at a heavy p-block element: unprecedented formation of a cationic bismuth carbamoyl. Chemical Science, 2019, 10, 4169-4176.	7.4	59
35	para-Selective Câ€“H Olefination of Aniline Derivatives via Pd/S,O-Ligand Catalysis. Journal of the American Chemical Society, 2019, 141, 6719-6725.	13.7	108
36	Open-shell jellium aromaticity in metal clusters. Chemical Communications, 2019, 55, 5559-5562.	4.1	15

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37	Probing Through-Space Polarâ^Ï€ Interactions in 2,6-Diarylphenols. Journal of Organic Chemistry, 2019, 84, 3632-3637.	3.2	11
38	Understanding the differences between iron and palladium in cross-coupling reactions. Physical Chemistry Chemical Physics, 2019, 21, 9651-9664.	2.8	12
39	52 GAMES WITH THE PERIODIC TABLE AND BEYOND. , 2019, , .		0
40	Recognition of shorter and longer trimethyllysine analogues by epigenetic reader proteins. Chemical Communications, 2018, 54, 2409-2412.	4.1	15
41	Doppelte CHâ€Aktivierung eines maskierten Bismutamidâ€Kations. Angewandte Chemie, 2018, 130, 3887-3891.	2.0	25
42	Double CH Activation of a Masked Cationic Bismuth Amide. Angewandte Chemie - International Edition, 2018, 57, 3825-3829.	13.8	66
43	Aromaticity Determines the Relative Stability of Kinked vs. Straight Topologies in Polycyclic Aromatic Hydrocarbons. Frontiers in Chemistry, 2018, 6, 561.	3.6	41
44	Rational design of nearâ€infrared absorbing organic dyes: Controlling the HOMOâ€“LUMO gap using quantitative molecular orbital theory. Journal of Computational Chemistry, 2018, 39, 2690-2696.	3.3	26
45	Covalent and Ionic Capacity of MOFs To Sorb Small Gas Molecules. Inorganic Chemistry, 2018, 57, 6981-6990.	4.0	55
46	B-DNA model systems in non-terran bio-solvents: implications for structure, stability and replication. Physical Chemistry Chemical Physics, 2017, 19, 16969-16978.	2.8	25
47	Kekulene: Structure, stability and nature of Hâ€¢â€¢â€¢H interactions in large PAHs. Molecular Astrophysics, 2017, 8, 19-26.	1.6	17
48	Nature of the Ruâ^'NO Coordination Bond: Kohnâ€“Sham Molecular Orbital and Energy Decomposition Analysis. ChemistryOpen, 2017, 6, 410-416.	1.9	11
49	Silyleneâ€Induced Reduction of [Mn₂(CO)₁₀]: Formation of a Fiveâ€Coordinate Silicon(IV) Complex with an Oâ€Bound [(OC)₄Mn=Mn(CO)₄]^{2â€“} Ligand. European Journal of Inorganic Chemistry, 2017, 2017, 186-191.	2.0	7
50	Testing the effectiveness of the isoelectronic substitution principle through the transformation of aromatic osmathiophene derivatives into their inorganic analogues. New Journal of Chemistry, 2017, 41, 1168-1178.	2.8	9
51	Stabilization of 2,6-Diarylanilinum Cation by Through-Space Cationâ^Ï€ Interactions. Journal of Organic Chemistry, 2017, 82, 9418-9424.	3.2	18
52	Formation of a Trifluorophosphane Platinum(II) Complex by Pâ^'F Bond Activation of Phosphorus Pentafluoride with a Pt⁰ Complex. Chemistry - A European Journal, 2017, 23, 5948-5952.	3.3	14
53	Reaction Mechanism and Regioselectivity of the Bingelâ€“Hirsch Addition of Dimethyl Bromomalonate to La@C₂v</sub>â€C₈₂. Chemistry - A European Journal, 2016, 22, 5953-5962.	3.3	23
54	Rules of Aromaticity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 321-335.	0.6	7

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55	Planar vs. three-dimensional X₆^{2â^'}, X₂Y₄^{2â^'}, and X₃Y₃^{2â^'} (X, Y = B,) Tj ETQq1 1 0.784314 Physical Chemistry Chemical Physics, 2016, 18, 21102-21110.	2.8	7
56	Exploring the validity of the Glidewellâ€"Lloyd extension of Clarâ€™s Ï€-sextet rule: assessment from polycyclic conjugated hydrocarbons. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	24
57	HÃ¼ckel's Rule of Aromaticity Categorizes Aromatic closo Boron Hydride Clusters. Chemistry - A European Journal, 2016, 22, 7437-7443.	3.3	103
58	Synthesis and Hydrolysis of Alkoxy(aminoalkyl)diorganylsilanes of the Formula Type R2(RO)Si(CH2)nNH2(R = Alkyl,n= 1-3): A Systematic Experimental and Computational Study. European Journal of Inorganic Chemistry, 2016, 2016, 1641-1659.	2.0	3
59	Complexes of adamantaneâ€based group 13 Lewis acids and superacids: Bonding analysis and thermodynamics of hydrogen splitting. Journal of Computational Chemistry, 2016, 37, 1355-1362.	3.3	10
60	Fmocâ€"RGDS based fibrils: atomistic details of their hierarchical assembly. Physical Chemistry Chemical Physics, 2016, 18, 1265-1278.	2.8	17
61	Octahedral aromaticity in ^{2S+1}A_{1g} X₆^q clusters (X =) Tj ETQq1 1 0.784314 rgBT	2.8	12
62	How carbo-benzenes fit molecules in their inner core as do biologic ion carriers?. Structural Chemistry, 2016, 27, 249-259.	2.0	6
63	Reactivity of the Donorâ€Stabilized Silylenes [iPrNC(Ph)NiPr]₂Si and [iPrNC(NiPr₂)NiPr]₂Si: Activation of CO₂ and CS₂. Chemistry - A European Journal, 2015, 21, 16665-16672.	3.3	49
64	Stable Fourâ€Coordinate Guanidinatosilicon(IV) Complexes with SiN 3 El Skeletons (El=S, Se, Te) and Sïï£¾El Double Bonds. Chemistry - A European Journal, 2015, 21, 14011-14021.	3.3	29
65	The Missing Entry in the Agosticâ€"Anagostic Series: Rh(I)â€"Î·¹-C Interactions in P(CH)P Pincer Complexes. Inorganic Chemistry, 2015, 54, 2960-2969.	4.0	46
66	Why 1,2-quinone derivatives are more stable than their 2,3-analogues?. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	16
67	Quantifying aromaticity with electron delocalisation measures. Chemical Society Reviews, 2015, 44, 6434-6451.	38.1	335
68	Chemical basis for the recognition of trimethyllysine by epigenetic reader proteins. Nature Communications, 2015, 6, 8911.	12.8	72
69	B-DNA structure and stability: the role of hydrogen bonding, Ï€â€"Ï€ stacking interactions, twist-angle, and solvation. Organic and Biomolecular Chemistry, 2014, 12, 4691-4700.	2.8	64
70	Ï€â€...Aromaticity and Threeâ€Dimensional Aromaticity: Two sides of the Same Coin?. Angewandte Chemie - International Edition, 2014, 53, 12191-12195.	13.8	242
71	Electroactive polymers for the detection of morphine. Journal of Polymer Research, 2014, 21, 1.	2.4	6
72	Aromaticity and Magnetic Properties of 1â€•and 2â€Indenones and Their Aza Derivatives. European Journal of Organic Chemistry, 2014, 2014, 5370-5377.	2.4	9

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73	Analysis of the Aromaticity of Five-Membered Heterometallacycles Containing Os, Ru, Rh, and Ir. Organometallics, 2014, 33, 1762-1773.	2.3	31
74	Aromatic properties of 8-hydroxyquinoline and its metal complexes. Open Chemistry, 2013, 11, 655-663.	1.9	8
75	Comparison between Alkalimetal and Group 11 Transition Metal Halide and Hydride Tetramers: Molecular Structure and Bonding. Journal of Physical Chemistry A, 2013, 117, 8026-8034.	2.5	9
76	Unraveling the Origin of the Relative Stabilities of Group 14 M₂N₂²⁺ (M, N = C, Si, Ge, Sn, and Pb) Isomer Clusters. Journal of Physical Chemistry A, 2013, 117, 10462-10469.	2.5	13
77	X₂Y₂ Isomers: Tuning Structure and Relative Stability through Electronegativity Differences (X = H, Li, Na, F, Cl, Br, I; Y = O, S, Se, Te). Inorganic Chemistry, 2013, 52, 2458-2465.	4.0	16
78	Analysis of the Relative Stabilities of Ortho, Meta, and Para MClY(XC₄H₄)(PH₃)₂ Heterometallabenzenes (M = Rh,) Tj ETQq0 0 0 rgBT/Overloc	2.9	37
79	Examining the formation of specific interactions between poly(3,4-ethylenedioxythiophene) and nucleotide bases. RSC Advances, 2013, 3, 2639.	3.6	7
80	Metalloaromaticity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 105-122.	14.6	105
81	A Simple Link between Hydrocarbon and Borohydride Chemistries. Chemistry - A European Journal, 2013, 19, 4169-4175.	3.3	40
82	Molecular structures of M2N22â^' (M and N = B, Al, and Ga) clusters using the gradient embedded genetic algorithm. Physical Chemistry Chemical Physics, 2012, 14, 14850.	2.8	18
83	On the electronic structure of second generation Hoveydaâ€“Grubbs alkene metathesis precursors. Computational and Theoretical Chemistry, 2012, 996, 57-67.	2.5	21
84	Solvent effects on hydrogen bonds in Watsonâ€“Crick, mismatched, and modified DNA base pairs. Computational and Theoretical Chemistry, 2012, 998, 57-63.	2.5	32
85	Properties of poly(3-halidethiophene)s. Physical Chemistry Chemical Physics, 2012, 14, 10050.	2.8	8
86	Open-shell spherical aromaticity: the 2N2 + 2N + 1 (with S = N + Â½) rule. Chemical Communications, 2011, 47, 11647.	4.1	49
87	A donor-functionalized, silyl-substituted pentadienyllithium: structural insight from experiment and theory. Chemical Communications, 2011, 47, 6162.	4.1	14
88	All-metal aromatic clusters M42â^' (M = B, Al, and Ga). Are Ï€-electrons distortive or not?. Physical Chemistry Chemical Physics, 2011, 13, 20673.	2.8	14
89	Understanding Conjugation and Hyperconjugation from Electronic Delocalization Measures. Journal of Physical Chemistry A, 2011, 115, 13104-13113.	2.5	30
90	Routes of Ï€-Electron Delocalization in 4-Substituted-1,2-benzoquinones. Journal of Organic Chemistry, 2011, 76, 550-556.	3.2	15

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91	An Analysis of the Isomerization Energies of 1,2-/1,3-Diazacyclobutadiene, Pyrazole/Imidazole, and Pyridazine/Pyrimidine with the Turn-Upside-Down Approach. Journal of Organic Chemistry, 2011, 76, 8913-8921.	3.2	43
92	Binding of 6-mer single-stranded homo-nucleotides to poly(3,4-ethylenedioxythiophene): specific hydrogen bonds with guanine. Soft Matter, 2011, 7, 9922.	2.7	13
93	Ab Initio Design of Chelating Ligands Relevant to Alzheimerâ€™s Disease: Influence of Metalloaromaticity. Journal of Physical Chemistry A, 2011, 115, 12659-12666.	2.5	20
94	Analysis of the Effects ofN-Substituents on Some Aspects of the Aromaticity of Imidazoles and Pyrazoles. Journal of Physical Chemistry A, 2011, 115, 8571-8577.	2.5	46
95	Selectivity in DNA replication. Interplay of steric shape, hydrogen bonds, Ï€-stacking and solvent effects. Chemical Communications, 2011, 47, 7326.	4.1	52
96	Aromaticity and electronic delocalization in all-metal clusters with single, double, and triple aromatic character. Theoretical Chemistry Accounts, 2011, 128, 419-431.	1.4	57
97	Theoretical studies on aromaticity of selected hydroxypyrones. Part 3#. Chelatoaromaticity phenomenon in metalcomplexes of hydroxypyrones. Journal of Physical Organic Chemistry, 2011, 24, 499-506.	1.9	16
98	Patterns of Ï€-electron delocalization in aromatic and antiaromatic organic compounds in the light of HÃ¼ckel's 4n + 2 rule. Physical Chemistry Chemical Physics, 2010, 12, 7126.	2.8	38
99	Adenine versus guanine quartets in aqueous solution: dispersion-corrected DFT study on the differences in Ï€-stacking and hydrogen-bonding behavior. Theoretical Chemistry Accounts, 2010, 125, 245-252.	1.4	123
100	A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity. Symmetry, 2010, 2, 1156-1179.	2.2	115
101	A Test to Evaluate the Performance of Aromaticity Descriptors in All-Metal and Semimetal Clusters. An Appraisal of Electronic and Magnetic Indicators of Aromaticity. Journal of Chemical Theory and Computation, 2010, 6, 1118-1130.	5.3	84
102	Examining the Planarity of Poly(3,4-ethylenedioxythiophene): Consideration of Self-Rigidification, Electronic, and Geometric Effects. Journal of Physical Chemistry A, 2010, 114, 1023-1028.	2.5	38
103	Alkali Metal Complexes of Silyl-Substitutedansa-(Tris)allyl Ligands: Metal-, Co-Ligand- and Substituent-Dependent Stereochemistry. European Journal of Inorganic Chemistry, 2009, 2009, 4157-4167.	2.0	15
104	Modeling the structureâ€property relationships of nanoneedles: A journey toward nanomedicine. Journal of Computational Chemistry, 2009, 30, 275-284.	3.3	76
105	Excess charge delocalization in organic and biological molecules: some theoretical notions. Theoretical Chemistry Accounts, 2009, 123, 29-40.	1.4	9
106	Aromaticity and Chemical Reactivity. , 2009, , .		5
107	Hypervalent versus Nonhypervalent Carbon in Nobleâ€Gas Complexes. Chemistry - A European Journal, 2008, 14, 6901-6911.	3.3	37
108	On the performance of some aromaticity indices: A critical assessment using a test set. Journal of Computational Chemistry, 2008, 29, 1543-1554.	3.3	261

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109	Analysis of HÃ¼ckelâ€™s [4n+ 2] Rule through Electronic Delocalization Measures. Journal of Physical Chemistry A, 2008, 112, 13231-13238.	2.5	38
110	Chapter 10 Electronic structure and reactivity of aromatic metal clusters. Theoretical and Computational Chemistry, 2007, 19, 203-218.	0.4	0
111	New Solids Based on B₁₂N₁₂ Fullerenes. Journal of Physical Chemistry C, 2007, 111, 13354-13360.	3.1	72
112	Aromaticity of Distorted Benzene Rings:â€‰ Exploring the Validity of Different Indicators of Aromaticity. Journal of Physical Chemistry A, 2007, 111, 4513-4521.	2.5	102
113	Didehydrophenanthrenes:â€‰ Structure, Singletâ^'Triplet Splitting, and Aromaticity. Journal of Physical Chemistry A, 2007, 111, 5063-5070.	2.5	39
114	Polycyclic Benzenoids:Â Why Kinked is More Stable than Straight. Journal of Organic Chemistry, 2007, 72, 1134-1142.	3.2	197
115	Aromaticity changes along the reaction coordinate connecting the cyclobutadiene dimer to cubane and the benzene dimer to hexaprismane. Structural Chemistry, 2007, 18, 773-783.	2.0	18
116	Role of Electron Density and Magnetic Couplings on the Nucleus-Independent Chemical Shift (NICS) Profiles of [2.2]Paracyclophane and Related Species. Journal of Organic Chemistry, 2006, 71, 1700-1702.	3.2	57
117	A trinuclear Pt(ii) compound with short Ptâ€“Ptâ€“Pt contacts. An analysis of the influence of Ï€â€“Ï€ stacking interactions on the strength and length of the Ptâ€“Pt bond. Dalton Transactions, 2006, , 1188-1196.	3.3	70
118	Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. Journal of Physical Chemistry A, 2006, 110, 12249-12258.	2.5	52
119	Bonding in Methylalkalimetals (CH3M)n(M = Li, Na, K;n= 1, 4). Agreement and Divergences between AIM and ELF Analysesâ€. Journal of Physical Chemistry B, 2006, 110, 7189-7198.	2.6	39
120	Are nucleus-independent (NICS) and 1H NMR chemical shifts good indicators of aromaticity in Ï€-stacked polyfluorenes?. Chemical Physics Letters, 2006, 428, 191-195.	2.6	33
121	Analysis of Electron Delocalization in Aromatic Systems:â€‰ Individual Molecular Orbital Contributions to Para-Delocalization Indexes (PDI). Journal of Physical Chemistry A, 2006, 110, 11569-11574.	2.5	28
122	Theoretical Evaluation of Electron Delocalization in Aromatic Molecules by Means of Atoms in Molecules (AIM) and Electron Localization Functional (ELF) Topological Approaches. ChemInform, 2006, 37, no.	0.0	0
123	Hydrogenâ€“Hydrogen Bonding in Planar Biphenyl, Predicted by Atoms-In-Molecules Theory, Does Not Exist. Chemistry - A European Journal, 2006, 12, 2889-2895.	3.3	314
124	A Model of the Chemical Bond Must Be Rooted in Quantum Mechanics, Provide Insight, and Possess Predictive Power. Chemistry - A European Journal, 2006, 12, 2902-2905.	3.3	216
125	Electron Fluctuation in Pericyclic and Pseudopericyclic Reactions. ChemPhysChem, 2006, 7, 111-113.	2.1	45
126	An analysis of the changes in aromaticity and planarity along the reaction path of the simplest Dielsâ€“Alder reaction. Exploring the validity of different indicators of aromaticity. Computational and Theoretical Chemistry, 2005, 727, 165-171.	1.5	59

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127	Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1â^'9). Journal of Organic Chemistry, 2005, 70, 2509-2521.	3.2	195
128	Aromaticity Analysis of Lithium Cation/ Ï€ Complexes of Aromatic Systems. ChemPhysChem, 2005, 6, 2552-2561.	2.1	46
129	Ab initio and DFT modeling of stereoselective deamination of aziridines by nitrosyl chloride. International Journal of Quantum Chemistry, 2005, 102, 139-146.	2.0	9
130	Assessment of Clar's aromatic Ï€-sextet rule by means of PDI, NICS and HOMA indicators of local aromaticity. Journal of Physical Organic Chemistry, 2005, 18, 785-791.	1.9	147
131	Theoretical Evaluation of Electron Delocalization in Aromatic Molecules by Means of Atoms in Molecules (AIM) and Electron Localization Function (ELF) Topological Approaches. Chemical Reviews, 2005, 105, 3911-3947.	47.7	661
132	Local Aromaticity of the Lowest-Lying Singlet States of [n]Acenes (n = 6â^'9). Journal of Physical Chemistry A, 2005, 109, 10629-10632.	2.5	68
133	Hydrogen bonding and aromaticity in the guanineâ€“cytosine base pair interacting with metal cations (Mâ€‰=â€‰Cu+, Ca2+and Cu2+). Molecular Physics, 2005, 103, 163-173.	1.7	32
134	Comment on the â€œNature of Bonding in the Thermal Cyclization of (Z)-1,2,4,6-Heptatetraene and Its Heterosubstituted Analoguesâ€• Journal of Physical Chemistry B, 2005, 109, 7591-7593.	2.6	17
135	Comparison of the AIM Delocalization Index and the Mayer and Fuzzy Atom Bond Orders. Journal of Physical Chemistry A, 2005, 109, 9904-9910.	2.5	169
136	Diastereoselective Synthesis of Fulleropyrrolidines from Suitably Functionalized Chiral Cyclobutanes. Journal of Organic Chemistry, 2005, 70, 6929-6932.	3.2	22
137	Relation between the Substituent Effect and Aromaticity. Journal of Organic Chemistry, 2004, 69, 6634-6640.	3.2	177
138	Analysis of electronic delocalization in buckminsterfullerene (C60). International Journal of Quantum Chemistry, 2004, 98, 361-366.	2.0	23
139	Discrepancy Between Common Local Aromaticity Measures in a Series of Carbazole Derivatives. ChemInform, 2004, 35, no.	0.0	0
140	Local Aromaticity of the Six-Membered Rings in Pyracylene. A Difficult Case for the NICS Indicator of Aromaticity. Journal of Organic Chemistry, 2004, 69, 7537-7542.	3.2	113
141	Ground and Low-Lying States of Cu2+â^'H2O. A Difficult Case for Density Functional Methods. Journal of Physical Chemistry A, 2004, 108, 6072-6078.	2.5	85
142	Discrepancy between common local aromaticity measures in a series of carbazole derivatives. Physical Chemistry Chemical Physics, 2004, 6, 314-318.	2.8	106
143	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes.. ChemInform, 2003, 34, no.	0.0	0
144	The Delocalization Index as an Electronic Aromaticity Criterion: Application to a Series of Planar Polycyclic Aromatic Hydrocarbons. Chemistry - A European Journal, 2003, 9, 400-406.	3.3	396

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145	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes. Chemistry - A European Journal, 2003, 9, 1113-1122.	3.3	125
146	Electron pairing analysis of the Fischer-type chromiumâ€“carbene complexes (CO)5Crî˜…C(X)R (X=H, OH,) Tj ETQq0 0 0 rgBT /Overlock	1.9	18
147	On the electron-pair nature of the hydrogen bond in the framework of the atoms in molecules theory. Chemical Physics Letters, 2003, 369, 248-255.	2.6	74
148	Nuclear magnetic resonance chemical shifts with the statistical average of orbital-dependent model potentials in Kohnâ€“Sham density functional theory. Journal of Chemical Physics, 2003, 118, 8584-8593.	3.0	48
149	Analysis of the effect of changing the a0 parameter of the Becke3-LYP hybrid functional on the transition state geometries and energy barriers in a series of prototypical reactions. Physical Chemistry Chemical Physics, 2002, 4, 722-731.	2.8	51
150	The calculation of electron localization and delocalization indices at the Hartree-Fock, density functional and post-Hartree-Fock levels of theory. Theoretical Chemistry Accounts, 2002, 107, 362-371.	1.4	187
151	Electron-pairing analysis from localization and delocalization indices in the framework of the atoms-in-molecules theory. Theoretical Chemistry Accounts, 2002, 108, 214-224.	1.4	175
152	New Insights in Chemical Reactivity by Means of Electron Pairing Analysis. Journal of Physical Chemistry A, 2001, 105, 2052-2063.	2.5	34
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