

Jordi Poater

List of Publications by Year in descending order

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156
papers

8,287
citations

53939

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165
docs citations

165
times ranked

5891
citing authors

#	ARTICLE	IF	CITATIONS
1	Path-dependency of energy decomposition analysis & the elusive nature of bonding. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 2344-2348.	1.3	27
2	C(<i>sp</i> ⁿ) ⁿ X (n=1-3) Bond Activation by Palladium. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	7
3	Probing the Lewis Acidity of Boronic Acids through Interactions with Arene Substituents. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	8
4	Rational design of iron catalysts for C - X bond activation. <i>Journal of Computational Chemistry</i> , 2022, , .	1.5	7
5	Aromaticity and Extrusion of Benzenoids Linked to [o]COSAN ⁺ : Clar Has the Answer. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	12
6	Reading and erasing of the phosphonium analogue of trimethyllysine by epigenetic proteins. <i>Communications Chemistry</i> , 2022, 5, .	2.0	5
7	C ⁿ X Bond Activation by Palladium: Steric Shielding versus Steric Attraction. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	11
8	Probing Noncovalent Interactions in [3,3]Metaparacyclophanes. <i>Journal of Organic Chemistry</i> , 2022, 87, 6087-6096.	1.7	2
9	Through-Space Stabilization of an Imidazolium Cation by Aromatic Rings. <i>Journal of Organic Chemistry</i> , 2022, 87, 7875-7883.	1.7	2
10	3D and 2D aromatic units behave like oil and water in the case of benzocarborane derivatives. <i>Nature Communications</i> , 2022, 13, .	5.8	23
11	Bismutamide als einfache Vermittler hochselektiver Pn ⁺ Pn ⁻ Radikal ⁻ Kupplungsreaktionen (Pn=N, P, As). <i>Angewandte Chemie</i> , 2021, 133, 6513-6518.	1.6	7
12	Bismuth Amides Mediate Facile and Highly Selective Pn ⁺ Pn ⁻ Radical ⁻ Coupling Reactions (Pn=N, P, As). <i>Angewandte Chemie - International Edition</i> , 2021, 60, 6441-6445.	7.2	36
13	The energy components of the extended transition state energy decomposition analysis are path functions: the case of water tetramer. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	8
14	Do Sulfonamides Interact with Aromatic Rings?. <i>Chemistry - A European Journal</i> , 2021, 27, 5721-5729.	1.7	7
15	Chelation enforcing a dual gold configuration in the catalytic hydroxyphenoxylation of alkynes. <i>Applied Organometallic Chemistry</i> , 2021, 35, e6362.	1.7	5
16	Pyrrrole and Pyridine in the Water Environment ⁺ Effect of Discrete and Continuum Solvation Models. <i>ACS Omega</i> , 2021, 6, 24693-24699.	1.6	4
17	Cage ⁿ · ⁿ · ⁿ · ⁿ Cage ⁿ Interaction: Boron Cluster-Based Noncovalent Bond and Its Applications in Solid-State Materials. <i>Jacs Au</i> , 2021, 1, 2047-2057.	3.6	5
18	The Chemical Bond: When Atom Size Instead of Electronegativity Difference Determines Trend in Bond Strength. <i>Chemistry - A European Journal</i> , 2021, 27, 15616-15622.	1.7	26

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19	Zwitterionic Aromaticity on Azulene Extrapolated to $\langle i \rangle$ carbo $\langle /i \rangle$ -Azulene. European Journal of Organic Chemistry, 2021, 2021, 6450-6458.	1.2	5
20	Phenoxylation of Alkynes through Mono- and Dual Activation Using Group 11 (Cu, Ag, Au) Catalysts. European Journal of Inorganic Chemistry, 2020, 2020, 1123-1134.	1.0	7
21	Activation Strain Analyses of Counterion and Solvent Effects on the Ion-Pair S _N 2 Reaction of and CH ₃ Cl. Journal of Computational Chemistry, 2020, 41, 317-327.	1.5	4
22	Distortion-Controlled Redshift of Organic Dye Molecules. Chemistry - A European Journal, 2020, 26, 2080-2093.	1.7	12
23	Probing Halogen \cdots versus CH \cdots Interactions in Molecular Balance. Organic Letters, 2020, 22, 7870-7873.	2.4	11
24	Analysis of the electronic delocalization in some isoelectronic analogues of B ₁₂ doped with beryllium and/or carbon. Physical Chemistry Chemical Physics, 2020, 22, 12245-12259.	1.3	12
25	Cyclopropenylidene phosphoranes: Rearrangement to Azetidinylidene-Methylphosphoniums. Journal of Organic Chemistry, 2020, 85, 7452-7458.	1.7	2
26	Mechanism of biomolecular recognition of trimethyllysine by the fluorinated aromatic cage of KDM5A PHD3 finger. Communications Chemistry, 2020, 3, .	2.0	13
27	Through-Space Polar Interactions in 2,6-Diarylthiophenols. ChemPhysChem, 2020, 21, 1080-1080.	1.0	0
28	The nido "Cage" Bond: A Non-covalent Interaction between Boron Clusters and Aromatic Rings and Its Applications. Angewandte Chemie, 2020, 132, 9103-9110.	1.6	7
29	The $\langle i \rangle$ nido "Cage" Bond: A Non-covalent Interaction between Boron Clusters and Aromatic Rings and Its Applications. Angewandte Chemie - International Edition, 2020, 59, 9018-9025.	7.2	32
30	Through-Space Polar Interactions in 2,6-Diarylthiophenols. ChemPhysChem, 2020, 21, 1092-1100.	1.0	9
31	Comparison of Molecular Recognition of Trimethyllysine and Trimethylthialysine by Epigenetic Reader Proteins. Molecules, 2020, 25, 1918.	1.7	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.	6.6	145
33	PyFrag 2019 "Automating the exploration and analysis of reaction mechanisms. Journal of Computational Chemistry, 2019, 40, 2227-2233.	1.5	57
34	Carbon monoxide insertion at a heavy p-block element: unprecedented formation of a cationic bismuth carbamoyl. Chemical Science, 2019, 10, 4169-4176.	3.7	59
35	$\langle i \rangle$ para-Selective C-H Olefination of Aniline Derivatives via Pd/S,O-Ligand Catalysis. Journal of the American Chemical Society, 2019, 141, 6719-6725.	6.6	108
36	Open-shell jellium aromaticity in metal clusters. Chemical Communications, 2019, 55, 5559-5562.	2.2	15

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37	Probing Through-Space Polar π - π Interactions in 2,6-Diarylphenols. <i>Journal of Organic Chemistry</i> , 2019, 84, 3632-3637.	1.7	11
38	Understanding the differences between iron and palladium in cross-coupling reactions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9651-9664.	1.3	12
39	52 GAMES WITH THE PERIODIC TABLE AND BEYOND. , 2019, , .		0
40	Recognition of shorter and longer trimethyllysine analogues by epigenetic reader proteins. <i>Chemical Communications</i> , 2018, 54, 2409-2412.	2.2	15
41	Doppelte CH δ -Aktivierung eines maskierten Bismutamid δ -Kations. <i>Angewandte Chemie</i> , 2018, 130, 3887-3891.	1.6	25
42	Double CH Activation of a Masked Cationic Bismuth Amide. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 3825-3829.	7.2	66
43	Aromaticity Determines the Relative Stability of Kinked vs. Straight Topologies in Polycyclic Aromatic Hydrocarbons. <i>Frontiers in Chemistry</i> , 2018, 6, 561.	1.8	41
44	Rational design of near-infrared absorbing organic dyes: Controlling the HOMO δ -LUMO gap using quantitative molecular orbital theory. <i>Journal of Computational Chemistry</i> , 2018, 39, 2690-2696.	1.5	26
45	Covalent and Ionic Capacity of MOFs To Sorb Small Gas Molecules. <i>Inorganic Chemistry</i> , 2018, 57, 6981-6990.	1.9	55
46	B-DNA model systems in non-terran bio-solvents: implications for structure, stability and replication. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 16969-16978.	1.3	25
47	Kekulene: Structure, stability and nature of H δ - δ -H interactions in large PAHs. <i>Molecular Astrophysics</i> , 2017, 8, 19-26.	1.7	17
48	Nature of the Ru δ -NO Coordination Bond: Kohn δ -Sham Molecular Orbital and Energy Decomposition Analysis. <i>ChemistryOpen</i> , 2017, 6, 410-416.	0.9	11
49	Silylene δ -Induced Reduction of [Mn ₂ (CO) ₁₀]: Formation of a Five δ -Coordinate Silicon(IV) Complex with an O δ -Bound [(OC) ₄ Mn=Mn(CO) ₄] ²⁺ Ligand. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 186-191.	1.0	7
50	Testing the effectiveness of the isoelectronic substitution principle through the transformation of aromatic osmathiophene derivatives into their inorganic analogues. <i>New Journal of Chemistry</i> , 2017, 41, 1168-1178.	1.4	9
51	Stabilization of 2,6-Diarylanilinium Cation by Through-Space Cation δ - π Interactions. <i>Journal of Organic Chemistry</i> , 2017, 82, 9418-9424.	1.7	18
52	Formation of a Trifluorophosphane Platinum(II) Complex by P δ -F Bond Activation of Phosphorus Pentafluoride with a Pt ⁰ Complex. <i>Chemistry - A European Journal</i> , 2017, 23, 5948-5952.	1.7	14
53	Reaction Mechanism and Regioselectivity of the Bingel δ -Hirsch Addition of Dimethyl Bromomalonate to La ₂ C ₂ δ -C ₈₂ . <i>Chemistry - A European Journal</i> , 2016, 22, 5953-5962.	1.7	23
54	Rules of Aromaticity. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2016, , 321-335.	0.6	7

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55	Planar vs. three-dimensional X_6^{2+} , $X_2Y_4^{2+}$, and $X_3Y_3^{2+}$ ($X, Y = B, Tl, Pb$) Physical Chemistry Chemical Physics, 2016, 18, 21102-21110.	1.3	170.784314
56	Exploring the validity of the Glidewell-Lloyd extension of Clar's sextet rule: assessment from polycyclic conjugated hydrocarbons. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	24
57	Hückel's Rule of Aromaticity Categorizes Aromatic Borene Boron Hydride Clusters. Chemistry - A European Journal, 2016, 22, 7437-7443.	1.7	103
58	Synthesis and Hydrolysis of Alkoxy(aminoalkyl)diorganylsilanes of the Formula Type $R_2(RO)Si(CH_2)_nNH_2$ ($R = \text{Alkyl}, n = 1-3$): A Systematic Experimental and Computational Study. European Journal of Inorganic Chemistry, 2016, 2016, 1641-1659.	1.0	3
59	Complexes of adamantane-based group 13 Lewis acids and superacids: Bonding analysis and thermodynamics of hydrogen splitting. Journal of Computational Chemistry, 2016, 37, 1355-1362.	1.5	10
60	Fmoc-RGDs based fibrils: atomistic details of their hierarchical assembly. Physical Chemistry Chemical Physics, 2016, 18, 1265-1278.	1.3	17
61	Octahedral aromaticity in $2S+1A_1g$ X_6^q clusters ($X = Tl, Pb, Bi, Po, At, Rn$) Physical Chemistry Chemical Physics, 2016, 18, 1265-1278.	1.3	120.784314
62	How carbo-benzenes fit molecules in their inner core as do biologic ion carriers?. Structural Chemistry, 2016, 27, 249-259.	1.0	6
63	Reactivity of the Donor-Stabilized Silylenes [$iPrNC(Ph)N(iPr)_2Si$ and [$iPrNC(N(iPr)_2)N(iPr)_2Si$: Activation of CO_2 and CS_2 . Chemistry - A European Journal, 2015, 21, 16665-16672.	1.7	49
64	Stable Four-Coordinate Guanidinosilicon(IV) Complexes with SiN_3 El Skeletons ($El = S, Se, Te$) and Si_2El_3 Double Bonds. Chemistry - A European Journal, 2015, 21, 14011-14021.	1.7	29
65	The Missing Entry in the Agostic-Anagostic Series: $Rh(I)^{1+}$ -C Interactions in $P(CH)_3$ Pincer Complexes. Inorganic Chemistry, 2015, 54, 2960-2969.	1.9	46
66	Why 1,2-quinone derivatives are more stable than their 2,3-analogues?. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	16
67	Quantifying aromaticity with electron delocalisation measures. Chemical Society Reviews, 2015, 44, 6434-6451.	18.7	335
68	Chemical basis for the recognition of trimethyllysine by epigenetic reader proteins. Nature Communications, 2015, 6, 8911.	5.8	72
69	B-DNA structure and stability: the role of hydrogen bonding, π - π stacking interactions, twist-angle, and solvation. Organic and Biomolecular Chemistry, 2014, 12, 4691-4700.	1.5	64
70	π -Aromaticity and Three-Dimensional Aromaticity: Two sides of the Same Coin?. Angewandte Chemie - International Edition, 2014, 53, 12191-12195.	7.2	242
71	Electroactive polymers for the detection of morphine. Journal of Polymer Research, 2014, 21, 1.	1.2	6
72	Aromaticity and Magnetic Properties of 1- and 2-Indenones and Their Aza Derivatives. European Journal of Organic Chemistry, 2014, 2014, 5370-5377.	1.2	9

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73	Analysis of the Aromaticity of Five-Membered Heterometallacycles Containing Os, Ru, Rh, and Ir. <i>Organometallics</i> , 2014, 33, 1762-1773.	1.1	31
74	Aromatic properties of 8-hydroxyquinoline and its metal complexes. <i>Open Chemistry</i> , 2013, 11, 655-663.	1.0	8
75	Comparison between Alkalimetal and Group 11 Transition Metal Halide and Hydride Tetramers: Molecular Structure and Bonding. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8026-8034.	1.1	9
76	Unraveling the Origin of the Relative Stabilities of Group 14 $M_2N_2^{2+}$ ($M, N = C, Si, Ge, Sn, \text{ and } Pb$) Isomer Clusters. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10462-10469.	1.1	13
77	X_2Y_2 Isomers: Tuning Structure and Relative Stability through Electronegativity Differences ($X = H, Li, Na, F, Cl, Br, I; Y = O, S, Se, Te$). <i>Inorganic Chemistry</i> , 2013, 52, 2458-2465.	1.9	16
78	Analysis of the Relative Stabilities of Ortho, Meta, and Para MCl_4H_4 (PH_3) $_2$ Heterometallabenzenes ($M = Rh$). <i>Tj ETQn 0 0 rgBk/Overlock</i>	1.0	7
79	Examining the formation of specific interactions between poly(3,4-ethylenedioxythiophene) and nucleotide bases. <i>RSC Advances</i> , 2013, 3, 2639.	1.7	7
80	Metalloaromaticity. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013, 3, 105-122.	6.2	105
81	A Simple Link between Hydrocarbon and Borohydride Chemistries. <i>Chemistry - A European Journal</i> , 2013, 19, 4169-4175.	1.7	40
82	Molecular structures of $M_2N_2^{2+}$ (M and $N = B, Al, \text{ and } Ga$) clusters using the gradient embedded genetic algorithm. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14850.	1.3	18
83	On the electronic structure of second generation Hoveyda's Grubbs alkene metathesis precursors. <i>Computational and Theoretical Chemistry</i> , 2012, 996, 57-67.	1.1	21
84	Solvent effects on hydrogen bonds in Watson-Crick, mismatched, and modified DNA base pairs. <i>Computational and Theoretical Chemistry</i> , 2012, 998, 57-63.	1.1	32
85	Properties of poly(3-halidethiophene)s. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10050.	1.3	8
86	Open-shell spherical aromaticity: the $2N_2 + 2N + 1$ (with $S = N + \hat{A}^{1/2}$) rule. <i>Chemical Communications</i> , 2011, 47, 11647.	2.2	49
87	A donor-functionalized, silyl-substituted pentadienyllithium: structural insight from experiment and theory. <i>Chemical Communications</i> , 2011, 47, 6162.	2.2	14
88	All-metal aromatic clusters M_4^{2+} ($M = B, Al, \text{ and } Ga$). Are π -electrons distortive or not?. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20673.	1.3	14
89	Understanding Conjugation and Hyperconjugation from Electronic Delocalization Measures. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13104-13113.	1.1	30
90	Routes of π -Electron Delocalization in 4-Substituted-1,2-benzoquinones. <i>Journal of Organic Chemistry</i> , 2011, 76, 550-556.	1.7	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. <i>Journal of Organic Chemistry</i> , 2011, 76, 8913-8921.	1.7	43
92	Binding of 6-mer single-stranded homo-nucleotides to poly(3,4-ethylenedioxythiophene): specific hydrogen bonds with guanine. <i>Soft Matter</i> , 2011, 7, 9922.	1.2	13
93	Ab Initio Design of Chelating Ligands Relevant to Alzheimer's Disease: Influence of Metalloaromaticity. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12659-12666.	1.1	20
94	Analysis of the Effects of N-Substituents on Some Aspects of the Aromaticity of Imidazoles and Pyrazoles. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8571-8577.	1.1	46
95	Selectivity in DNA replication. Interplay of steric shape, hydrogen bonds, π -stacking and solvent effects. <i>Chemical Communications</i> , 2011, 47, 7326.	2.2	52
96	Aromaticity and electronic delocalization in all-metal clusters with single, double, and triple aromatic character. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 419-431.	0.5	57
97	Theoretical studies on aromaticity of selected hydroxypyrones. Part 3#. Chelatoaromaticity phenomenon in metalcomplexes of hydroxypyrones. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 499-506.	0.9	16
98	Patterns of π -electron delocalization in aromatic and antiaromatic organic compounds in the light of Hückel's $4n + 2$ rule. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7126.	1.3	38
99	Adenine versus guanine quartets in aqueous solution: dispersion-corrected DFT study on the differences in π -stacking and hydrogen-bonding behavior. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 245-252.	0.5	123
100	A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity. <i>Symmetry</i> , 2010, 2, 1156-1179.	1.1	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. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1118-1130.	2.3	84
102	Examining the Planarity of Poly(3,4-ethylenedioxythiophene): Consideration of Self-Rigidification, Electronic, and Geometric Effects. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1023-1028.	1.1	38
103	Alkali Metal Complexes of Silyl-Substitutedansa-(Tris)allyl Ligands: Metal-, Co-Ligand- and Substituent-Dependent Stereochemistry. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 4157-4167.	1.0	15
104	Modeling the structure-property relationships of nanoneedles: A journey toward nanomedicine. <i>Journal of Computational Chemistry</i> , 2009, 30, 275-284.	1.5	76
105	Excess charge delocalization in organic and biological molecules: some theoretical notions. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 29-40.	0.5	9
106	Aromaticity and Chemical Reactivity. , 2009, , .		5
107	Hypervalent versus Nonhypervalent Carbon in Noble Gas Complexes. <i>Chemistry - A European Journal</i> , 2008, 14, 6901-6911.	1.7	37
108	On the performance of some aromaticity indices: A critical assessment using a test set. <i>Journal of Computational Chemistry</i> , 2008, 29, 1543-1554.	1.5	261

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109	Analysis of Hückel's [4n+2] Rule through Electronic Delocalization Measures. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13231-13238.	1.1	38
110	Chapter 10 Electronic structure and reactivity of aromatic metal clusters. <i>Theoretical and Computational Chemistry</i> , 2007, 19, 203-218.	0.2	0
111	New Solids Based on B ₁₂ N ₁₂ Fullerenes. <i>Journal of Physical Chemistry C</i> , 2007, 111, 13354-13360.	1.5	72
112	Aromaticity of Distorted Benzene Rings: Exploring the Validity of Different Indicators of Aromaticity. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4513-4521.	1.1	102
113	Didehydrophenanthrenes: Structure, Singlet-Triplet Splitting, and Aromaticity. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5063-5070.	1.1	39
114	Polycyclic Benzenoids: Why Kinked is More Stable than Straight. <i>Journal of Organic Chemistry</i> , 2007, 72, 1134-1142.	1.7	197
115	Aromaticity changes along the reaction coordinate connecting the cyclobutadiene dimer to cubane and the benzene dimer to hexaprismane. <i>Structural Chemistry</i> , 2007, 18, 773-783.	1.0	18
116	Role of Electron Density and Magnetic Couplings on the Nucleus-Independent Chemical Shift (NICS) Profiles of [2.2]Paracyclophane and Related Species. <i>Journal of Organic Chemistry</i> , 2006, 71, 1700-1702.	1.7	57
117	A trinuclear Pt(II) compound with short Pt-Pt contacts. An analysis of the influence of π - π stacking interactions on the strength and length of the Pt-Pt bond. <i>Dalton Transactions</i> , 2006, , 1188-1196.	1.6	70
118	Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12249-12258.	1.1	52
119	Bonding in Methylalkalimetal (CH ₃ M) _n (M = Li, Na, K; n = 1, 4). Agreement and Divergences between AIM and ELF Analyses. <i>Journal of Physical Chemistry B</i> , 2006, 110, 7189-7198.	1.2	39
120	Are nucleus-independent (NICS) and ¹ H NMR chemical shifts good indicators of aromaticity in π -stacked polyfluorenes?. <i>Chemical Physics Letters</i> , 2006, 428, 191-195.	1.2	33
121	Analysis of Electron Delocalization in Aromatic Systems: Individual Molecular Orbital Contributions to Para-Delocalization Indexes (PDI). <i>Journal of Physical Chemistry A</i> , 2006, 110, 11569-11574.	1.1	28
122	Theoretical Evaluation of Electron Delocalization in Aromatic Molecules by Means of Atoms in Molecules (AIM) and Electron Localization Functional (ELF) Topological Approaches. <i>ChemInform</i> , 2006, 37, no.	0.1	0
123	Hydrogen-Hydrogen Bonding in Planar Biphenyl, Predicted by Atoms-In-Molecules Theory, Does Not Exist. <i>Chemistry - A European Journal</i> , 2006, 12, 2889-2895.	1.7	314
124	A Model of the Chemical Bond Must Be Rooted in Quantum Mechanics, Provide Insight, and Possess Predictive Power. <i>Chemistry - A European Journal</i> , 2006, 12, 2902-2905.	1.7	216
125	Electron Fluctuation in Pericyclic and Pseudopericyclic Reactions. <i>ChemPhysChem</i> , 2006, 7, 111-113.	1.0	45
126	An analysis of the changes in aromaticity and planarity along the reaction path of the simplest Diels-Alder reaction. Exploring the validity of different indicators of aromaticity. <i>Computational and Theoretical Chemistry</i> , 2005, 727, 165-171.	1.5	59

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127	Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1~9). <i>Journal of Organic Chemistry</i> , 2005, 70, 2509-2521.	1.7	195
128	Aromaticity Analysis of Lithium Cation/π Complexes of Aromatic Systems. <i>ChemPhysChem</i> , 2005, 6, 2552-2561.	1.0	46
129	Ab initio and DFT modeling of stereoselective deamination of aziridines by nitrosyl chloride. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 139-146.	1.0	9
130	Assessment of Clar's aromatic sextet rule by means of PDI, NICS and HOMA indicators of local aromaticity. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 785-791.	0.9	147
131	Theoretical Evaluation of Electron Delocalization in Aromatic Molecules by Means of Atoms in Molecules (AIM) and Electron Localization Function (ELF) Topological Approaches. <i>Chemical Reviews</i> , 2005, 105, 3911-3947.	23.0	661
132	Local Aromaticity of the Lowest-Lying Singlet States of [n]Acenes (n = 6~9). <i>Journal of Physical Chemistry A</i> , 2005, 109, 10629-10632.	1.1	68
133	Hydrogen bonding and aromaticity in the guanine-cytosine base pair interacting with metal cations (M=Cu+, Ca2+ and Cu2+). <i>Molecular Physics</i> , 2005, 103, 163-173.	0.8	32
134	Comment on the Nature of Bonding in the Thermal Cyclization of (Z)-1,2,4,6-Heptatetraene and Its Heterosubstituted Analogues. <i>Journal of Physical Chemistry B</i> , 2005, 109, 7591-7593.	1.2	17
135	Comparison of the AIM Delocalization Index and the Mayer and Fuzzy Atom Bond Orders. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9904-9910.	1.1	169
136	Diastereoselective Synthesis of Fulleropyrrolidines from Suitably Functionalized Chiral Cyclobutanes. <i>Journal of Organic Chemistry</i> , 2005, 70, 6929-6932.	1.7	22
137	Relation between the Substituent Effect and Aromaticity. <i>Journal of Organic Chemistry</i> , 2004, 69, 6634-6640.	1.7	177
138	Analysis of electronic delocalization in buckminsterfullerene (C60). <i>International Journal of Quantum Chemistry</i> , 2004, 98, 361-366.	1.0	23
139	Discrepancy Between Common Local Aromaticity Measures in a Series of Carbazole Derivatives. <i>ChemInform</i> , 2004, 35, no.	0.1	0
140	Local Aromaticity of the Six-Membered Rings in Pyracylene. A Difficult Case for the NICS Indicator of Aromaticity. <i>Journal of Organic Chemistry</i> , 2004, 69, 7537-7542.	1.7	113
141	Ground and Low-Lying States of Cu2+·H2O. A Difficult Case for Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6072-6078.	1.1	85
142	Discrepancy between common local aromaticity measures in a series of carbazole derivatives. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 314-318.	1.3	106
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