Miquel SolÃ

List of Publications by Year
in descending order

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471 papers	20,593 citations	10389 72 h-index	20358 116 g-index
515 all docs	515 docs citations	515 times ranked	11286 citing authors

#	Article	IF	Citations
1	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
2	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
3	The aromatic fluctuation index (FLU): A new aromaticity index based on electron delocalization. Journal of Chemical Physics, 2005, 122, 014109.	3.0	396
4	Theoretical Studies of Some Transition-Metal-Mediated Reactions of Industrial and Synthetic Importance. Chemical Reviews, 2000, 100, 439-494.	47.7	371
5	Quantifying aromaticity with electron delocalisation measures. Chemical Society Reviews, 2015, 44, 6434-6451.	38.1	335
6	Forty years of Clar's aromatic Ï€-sextet rule. Frontiers in Chemistry, 2013, 1, 22.	3.6	332
7	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
8	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
9	Ï€â€…Aromaticity and Threeâ€Dimensional Aromaticity: Two sides of the Same Coin?. Angewandte Chemie - International Edition, 2014, 53, 12191-12195.	13.8	242
10	Nucleophilic Aryl Fluorination and Aryl Halide Exchange Mediated by a Cu^I/Cu^{III} Catalytic Cycle. Journal of the American Chemical Society, 2011, 133, 19386-19392.	13.7	232
11	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
12	Chemical bonding in transition metal carbene complexes. Journal of Organometallic Chemistry, 2005, 690, 6178-6204.	1.8	206
13	Electron sharing indexes at the correlated level. Application to aromaticity calculations. Faraday Discussions, 2007, 135, 325-345.	3.2	203
14	Polycyclic Benzenoids:Â Why Kinked is More Stable than Straight. Journal of Organic Chemistry, 2007, 72, 1134-1142.	3.2	197
15	Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1â^'9). Journal of Organic Chemistry, 2005, 70, 2509-2521.	3.2	195
16	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
17	Relation between the Substituent Effect and Aromaticity. Journal of Organic Chemistry, 2004, 69, 6634-6640.	3.2	177
18	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

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19	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
20	Nucleus-independent chemical shift (NICS) profiles in a series of monocyclic planar inorganic compounds. Journal of Organometallic Chemistry, 2006, 691, 4359-4366.	1.8	155
21	On the Validity of the Maximum Hardness Principle and the Minimum Electrophilicity Principle during Chemical Reactions. Journal of Physical Chemistry A, 2013, 117, 1843-1852.	2.5	152
22	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
23	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
24	The role of electronic delocalization in transition metal complexes from the electron localization function and the quantum theory of atoms in molecules viewpoints. Coordination Chemistry Reviews, 2009, 253, 647-665.	18.8	141
25	Electron localization function at the correlated level. Journal of Chemical Physics, 2006, 125, 024301.	3.0	135
26	Ab initio and DFT benchmark study for nucleophilic substitution at carbon (SN2@C) and silicon (SN2@Si). Journal of Computational Chemistry, 2005, 26, 1497-1504.	3.3	133
27	Importance of the Basis Set for the Spin-State Energetics of Iron Complexes. Journal of Physical Chemistry A, 2008, 112, 6384-6391.	2.5	131
28	Facile Câˆ'H Bond Cleavage via a Proton-Coupled Electron Transfer Involving a Câˆ'HÂ·Â·Â·Cu^{II}Interaction. Journal of the American Chemical Society, 2010, 132, 12299-12306.	13.7	131
29	The reactivity of endohedral fullerenes. What can be learnt from computational studies?. Physical Chemistry Chemical Physics, 2011, 13, 3585-3603.	2.8	128
30	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes. Chemistry - A European Journal, 2003, 9, 1113-1122.	3.3	125
31	Mechanistic Studies of Transition-Metal-Catalyzed [2 + 2 + 2] Cycloaddition Reactions. Chemical Reviews, 2021, 121, 1894-1979.	47.7	125
32	Analysis of solvent effects on the Menshutkin reaction. Journal of the American Chemical Society, 1991, 113, 2873-2879.	13.7	123
33	Density Functional Study of the [2+2]- and [2+3]-Cycloaddition Mechanisms for the Osmium-Catalyzed Dihydroxylation of Olefins. Organometallics, 1997, 16, 13-19.	2.3	122
34	Properties of Aromaticity Indices Based on the One-Electron Density Matrix. Journal of Physical Chemistry A, 2007, 111, 6521-6525.	2.5	118
35	Dispersion Corrections Essential for the Study of Chemical Reactivity in Fullerenes. Journal of Physical Chemistry A, 2011, 115, 3491-3496.	2.5	117
36	Electron delocalization and aromaticity in low-lying excited states of archetypal organic compounds. Physical Chemistry Chemical Physics, 2011, 13, 20690.	2.8	116

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37	A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity. Symmetry, 2010, 2, 1156-1179.	2.2	115
38	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2010, 6, 2736-2742.	5.3	115
39	The electron density of delocalized bonds (EDDB) applied for quantifying aromaticity. Physical Chemistry Chemical Physics, 2017, 19, 28970-28981.	2.8	114
40	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
41	A new all-round density functional based on spin states and S[sub N]2 barriers. Journal of Chemical Physics, 2009, 131, 094103.	3.0	113
42	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	3.3	113
43	On the Validity of the Maximum Hardness and Minimum Polarizability Principles for Nontotally Symmetric Vibrations. Journal of the American Chemical Society, 2001, 123, 7951-7952.	13.7	112
44	Interplay between Intramolecular Resonance-Assisted Hydrogen Bonding and Aromaticity in o-Hydroxyaryl Aldehydes. Journal of Organic Chemistry, 2006, 71, 5241-5248.	3.2	110
45	Why Aromaticity Is a Suspicious Concept? Why?. Frontiers in Chemistry, 2017, 5, 22.	3.6	108
46	Discrepancy between common local aromaticity measures in a series of carbazole derivatives. Physical Chemistry Chemical Physics, 2004, 6, 314-318.	2.8	106
47	Fine-Tuning the Electronic Properties of Highly Stable Organometallic CuIII Complexes Containing Monoanionic Macrocyclic Ligands. Chemistry - A European Journal, 2005, 11, 5146-5156.	3.3	106
48	Basis set and electron correlation effects on ab initio electronic and vibrational nonlinear optical properties of conjugated organic molecules. Journal of Chemical Physics, 2003, 118, 711-718.	3.0	105
49	Metalloaromaticity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 105-122.	14.6	105
50	HÃ¼ckel's Rule of Aromaticity Categorizes Aromatic closo Boron Hydride Clusters. Chemistry - A European Journal, 2016, 22, 7437-7443.	3.3	103
51	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
52	Why Do Cycloaddition Reactions Involving C₆₀ Prefer [6,6] over [5,6] Bonds?. Chemistry - A European Journal, 2013, 19, 7416-7422.	3.3	100
53	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
54	Molecular Structure and Bonding of Copper Cluster Monocarbonyls CunCO (n= 1â˜9). Journal of Physical Chemistry B, 2006, 110, 6526-6536.	2.6	97

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55	The role of aromaticity in determining the molecular structure and reactivity of (endohedral) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf	38.1	97
56	Mechanism of the Addition Reaction of Alkyl Azides to [60]Fullerene and the Subsequent N2Extrusion to Form Monoimino-[60]fullerenes. Journal of Organic Chemistry, 2001, 66, 433-442.	3.2	91
57	Energy landscapes of nucleophilic substitution reactions: A comparison of density functional theory and coupled cluster methods. Journal of Computational Chemistry, 2007, 28, 1551-1560.	3.3	89
58	E2 and S_N2 Reactions of X^{â^'} + CH₃CH₂X (X = F, Cl); an ab Initio and DFT Benchmark Study. Journal of Chemical Theory and Computation, 2008, 4, 929-940.	5.3	86
59	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
60	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
61	Not All That Has a Negative NICS Is Aromatic: The Case of the H-Bonded Cyclic Trimer of HF. Journal of Chemical Theory and Computation, 2010, 6, 1131-1135.	5.3	81
62	Molecular Structure and Bond Characterization of the Fischer-Type Chromiumâ^'Carbene Complexes (CO)5CrC(X)R (X = H, OH, OCH3, NH2, NHCH3 and R = H, CH3, CHCH2, Ph, Câ‹®CH). Organometallics, 2002, 21, 4182-4191.	2.3	80
63	Theoretical Evaluation of Solvent Effects on the Conformational and Tautomeric Equilibria of 2-(2â€˜-Hydroxyphenyl)benzimidazole and on Its Absorption and Fluorescence Spectra. Journal of Physical Chemistry A, 1999, 103, 4525-4532.	2.5	79
64	Excited-State Intramolecular Proton Transfer and Rotamerism of 2-(2â€˜-hydroxyvinyl)benzimidazole and 2-(2â€˜-hydroxyphenyl)imidazole. Journal of Physical Chemistry A, 1999, 103, 4413-4420.	2.5	78
65	Electronic and Vibrational Nonlinear Optical Properties of Five Representative Electrides. Journal of Chemical Theory and Computation, 2012, 8, 2688-2697.	5.3	78
66	Cyclo[18]carbon: the smallest all-carbon electron acceptor. Chemical Communications, 2020, 56, 352-355.	4.1	78
67	Are the maximum hardness and minimum polarizability principles always obeyed in nontotally symmetric vibrations?. Journal of Chemical Physics, 2002, 117, 10561-10570.	3.0	77
68	Aromaticity Measures from Fuzzy-Atom Bond Orders (FBO). The Aromatic Fluctuation (FLU) and the para-Delocalization (PDI) Indexes. Journal of Physical Chemistry A, 2006, 110, 5108-5113.	2.5	76
69	Modeling the structureâ€property relationships of nanoneedles: A journey toward nanomedicine. Journal of Computational Chemistry, 2009, 30, 275-284.	3.3	76
70	The Dielsâ^'Alder Reaction on Endohedral Y₃N@C₇₈: The Importance of the Fullerene Strain Energy. Journal of the American Chemical Society, 2009, 131, 129-139.	13.7	76
71	Chemical Reactivity of D3h C78 (Metallo)Fullerene: Regioselectivity Changes Induced by Sc3N Encapsulation. Journal of the American Chemical Society, 2008, 130, 6206-6214.	13.7	75
72	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

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73	Ab initio benchmark study for the oxidative addition of CH4 to Pd: Importance of basis-set flexibility and polarization. Journal of Chemical Physics, 2004, 121, 9982-9992.	3.0	73
74	New Solids Based on B₁₂N₁₂ Fullerenes. Journal of Physical Chemistry C, 2007, 111, 13354-13360.	3.1	72
75	Foundations and recent developments on molecular quantum similarity. Topics in Current Chemistry, 1995, , 31-62.	4.0	72
76	Reactivity Patterns of (Protonated) Compoundâ€…II and Compoundâ€…I of Cytochrome P450: Which is the Better Oxidant?. Chemistry - A European Journal, 2017, 23, 6406-6418.	3.3	71
77	Ab initio study of the hydration of carbon dioxide by carbonic anhydrase. A comparison between the Lipscomb and Lindskog mechanisms. Journal of the American Chemical Society, 1992, 114, 869-877.	13.7	70
78	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
79	Oxidative addition of the ethane Cï£¿C bond to Pd. Anab initiobenchmark and DFT validation study. Journal of Computational Chemistry, 2005, 26, 1006-1020.	3.3	69
80	The role of the longâ€range exchange corrections in the description of electron delocalization in aromatic species. Journal of Computational Chemistry, 2017, 38, 1640-1654.	3.3	69
81	Mechanism of the Manganese-Pincer-Catalyzed Acceptorless Dehydrogenative Coupling of Nitriles and Alcohols. Journal of the American Chemical Society, 2019, 141, 2398-2403.	13.7	69
82	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
83	Interplay between Intramolecular Resonance-Assisted Hydrogen Bonding and Local Aromaticity. II. 1,3-Dihydroxyaryl-2-aldehydes. Journal of Organic Chemistry, 2009, 74, 2059-2066.	3.2	68
84	Density Functional Study of the [2+2+2] Cyclotrimerization of Acetylene Catalyzed by Wilkinsonâ€™s Catalyst, RhCl(PPh₃)₃. Organometallics, 2010, 29, 562-569.	2.3	68
85	On the existence and characterization of molecular electrides. Chemical Communications, 2015, 51, 4865-4868.	4.1	68
86	Mechanism of the Suzukiâ€“Miyaura Cross-Coupling Reaction Mediated by [Pd(NHC)(allyl)Cl] Precatalysts. Organometallics, 2017, 36, 2088-2095.	2.3	68
87	Acidic Câ€“H Bond as a Proton Donor in Excited State Intramolecular Proton Transfer Reactions. Journal of Chemical Theory and Computation, 2015, 11, 1046-1054.	5.3	65
88	Theoretical Study of Dielsâ˜’Alder Cycloadditions of Butadiene to C70. An Insight into the Chemical Reactivity of C70as Compared to C60. The Journal of Physical Chemistry, 1996, 100, 7449-7454.	2.9	64
89	Computational methods to predict the reactivity of nanoparticles through structureâ€“property relationships. Expert Opinion on Drug Delivery, 2010, 7, 295-305.	5.0	64
90	A Theoretical Study of Steric and Electronic Effects in the Rhodium-Catalyzed Carbonylation Reactions. Journal of the American Chemical Society, 2001, 123, 12294-12302.	13.7	63

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91	Dielsâ^'Alder Reaction between Cyclopentadiene and C₆₀: An Analysis of the Performance of the ONIOM Method for the Study of Chemical Reactivity in Fullerenes and Nanotubes. Journal of Physical Chemistry A, 2009, 113, 9721-9726.	2.5	63
92	The Hammond Postulate and the Principle of Maximum Hardness in Some Intramolecular Rearrangement Reactions. Journal of Physical Chemistry A, 1999, 103, 8847-8852.	2.5	62
93	Complete Mechanism of Ïƒ* Intramolecular Aromatic Hydroxylation through O₂Activation by a Macrocyclic Dicopper(I) Complex. Journal of the American Chemical Society, 2008, 130, 17710-17717.	13.7	62
94	Copper(II) Hexaaza Macrocyclic Binuclear Complexes Obtained from the Reaction of Their Copper(I) Derivates and Molecular Dioxygen. Inorganic Chemistry, 2006, 45, 3569-3581.	4.0	61
95	A dissected ring current model for assessing magnetic aromaticity: A general approach for both organic and inorganic rings. Journal of Computational Chemistry, 2011, 32, 2422-2431.	3.3	61
96	Basis set and electron correlation effects on initial convergence for vibrational nonlinear optical properties of conjugated organic molecules. Journal of Chemical Physics, 2004, 120, 6346-6355.	3.0	60
97	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
98	Regioselective Intramolecular Pauson-Khand Reactions of C60: An Electrochemical Study and Theoretical Underpinning. Chemistry - A European Journal, 2005, 11, 2716-2729.	3.3	58
99	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
100	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
101	On the Mechanism of the Thermal Retrocycloaddition of Pyrrolidinofullerenes (Retroâ€Prato) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf	3.3	56
102	Reaction Mechanisms for Graphene and Carbon Nanotube Fluorination. Journal of Physical Chemistry C, 2010, 114, 3340-3345.	3.1	56
103	Theoretical Study of Gas-Phase Reactions of Fe(CO)5 with OH- and Their Relevance for the Water Gas Shift Reaction. Organometallics, 1999, 18, 2801-2812.	2.3	55
104	Maximum Aromaticity as a Guiding Principle for the Most Suitable Hosting Cages in Endohedral Metallofullerenes. Angewandte Chemie - International Edition, 2013, 52, 9275-9278.	13.8	55
105	Can Bairdâ€™s and Clarâ€™s Rules Combined Explain Triplet State Energies of Polycyclic Conjugated Hydrocarbons with Fused 4nÏ€- and (4n + 2)Ï€-Rings?. Journal of Organic Chemistry, 2017, 82, 6327-6340.	3.2	55
106	Aromaticity rules. Nature Chemistry, 2022, 14, 585-590.	13.6	55
107	Use of ab Initio Quantum Molecular Similarities as an Interpretative Tool for the Study of Chemical Reactions. Journal of the American Chemical Society, 1994, 116, 5909-5915.	13.7	54
108	A comparative analysis by means of quantum molecular similarity measures of density distributions derived from conventional ab initio and density functional methods. Journal of Chemical Physics, 1996, 104, 636-647.	3.0	54

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109	The Exohedral Dielsâ€“Alder Reactivity of the Titanium Carbide Endohedral Metallofullerene Ti₂C₂@D₃h</sub>â€“₇₈: Comparison with D₃h</sub>â€“₇₈ and M₃N@D₃h</sub>â€“₇₈ (M=Sc and Y) Reactivity. Chemistry - A European Journal, 2012, 18, 7141-7154.	3.3	54
110	Thermal [2+2] Intramolecular Cycloadditions of Fuller-1,6-enynes. Angewandte Chemie - International Edition, 2006, 45, 1439-1442.	13.8	53
111	Mechanistic Insights into the Chemistry of Ru(II) Complexes Containing Cl and DMSO Ligands. Inorganic Chemistry, 2007, 46, 10707-10716.	4.0	53
112	Theoretical investigation of the relative stabilities ofXSSXandX2SS isomers (X= F, Cl, H, and CH3). Journal of Computational Chemistry, 1995, 16, 465-477.	3.3	52
113	Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. Journal of Physical Chemistry A, 2006, 110, 12249-12258.	2.5	52
114	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
115	The linear response kernel of conceptual DFT as a measure of aromaticity. Physical Chemistry Chemical Physics, 2012, 14, 3960.	2.8	51
116	Molecular Size and Pyramidalization: Two Keys for Understanding the Reactivity of Fullerenes. The Journal of Physical Chemistry, 1995, 99, 10752-10758.	2.9	50
117	Cycloaddition of CO₂ to epoxides by highly nucleophilic 4-aminopyridines: establishing a relationship between carbon basicity and catalytic performance by experimental and DFT investigations. Organic Chemistry Frontiers, 2021, 8, 613-627.	4.5	50
118	An AM1 study of the reactivity of buckminsterfullerene (C60) in a Diels-Alder model reaction. Chemical Physics Letters, 1994, 231, 325-330.	2.6	49
119	Theoretical Study on Acetaldehyde and Ethanol Elimination from the Hydrogenation of CH3(O)CCo(CO)3. Organometallics, 1996, 15, 2611-2618.	2.3	49
120	Rhodium(I)â€Catalysed Intramolecular [2+2+2] Cyclotrimerisations of 15â€, 20â€•and 25â€Membered Azamacrocycles: Experimental and Theoretical Mechanistic Studies. Chemistry - A European Journal, 2009, 15, 5289-5300.	3.3	49
121	On the Mechanism of Action of Fullerene Derivatives in Superoxide Dismutation. Chemistry - A European Journal, 2010, 16, 3207-3214.	3.3	49
122	Open-shell spherical aromaticity: the 2N2 + 2N + 1 (with S = N + Â½) rule. Chemical Communications, 2011, 47, 11647.	4.1	49
123	Full Exploration of the Dielsâ€“Alder Cycloaddition on Metallofullerenes M₃N@C₈₀ (M=Sc, Lu, Gd): The D₅h</sub> versus I_h Isomer and the Influence of the Metal Cluster. Chemistry - A European Journal, 2012, 18, 8944-8956.	3.3	49
124	Electron Delocalization in Planar Metallacycles: HÃ¼ckel or MÃ¶bius Aromatic?. ChemistryOpen, 2019, 8, 219-227.	1.9	49
125	Covalency in Highly Polar Bonds. Structure and Bonding of Methylalkalimetal Oligomers (CH3M)n (M) Tj ETQq1 1 0.784314 rgBT /Ov	5.3	48
126	On the quality of the hardness kernel and the Fukui function to evaluate the global hardness. Journal of Computational Chemistry, 2007, 28, 574-583.	3.3	48

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127	Initiating Electron Transfer in Doubly Curved Nanographene Upon Supramolecular Complexation of C₆₀. Angewandte Chemie - International Edition, 2022, 61, .	13.8	48
128	Spin-State-Corrected Gaussian-Type Orbital Basis Sets. Journal of Physical Chemistry A, 2010, 114, 7191-7197.	2.5	47
129	One Century of Physical Organic Chemistry: The Menshutkin Reaction. Progress in Physical Organic Chemistry, 0, , 1-182.	1.2	47
130	On the calculation ofab initioquantum molecular similarities for large systems: Fitting the electron density. Journal of Computational Chemistry, 1994, 15, 1113-1120.	3.3	46
131	Aromaticity Analysis of Lithium Cation/ Ï€ Complexes of Aromatic Systems. ChemPhysChem, 2005, 6, 2552-2561.	2.1	46
132	Electron delocalization and aromaticity measures within the HÃ¼ckel molecular orbital method. Computational and Theoretical Chemistry, 2007, 811, 3-11.	1.5	46
133	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
134	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
135	Electron Fluctuation in Pericyclic and Pseudopericyclic Reactions. ChemPhysChem, 2006, 7, 111-113.	2.1	45
136	Reactivity and Regioselectivity of Noble Gas Endohedral Fullerenes Ng@C₆₀ and Ng₂@C₆₀ (Ng=Heâ€“Xe). Chemistry - A European Journal, 2009, 15, 13111-13123.	3.3	45
137	Understanding the Reactivity of Endohedral Metallofullerenes: C₇₈ versus Sc₃N@C₇₈. Chemistry - A European Journal, 2015, 21, 5760-5768.	3.3	45
138	Electrochemical control of the regioselectivity in the exohedral functionalization of C60: the role of aromaticity. Chemical Communications, 2013, 49, 1220.	4.1	44
139	Initial convergence of the perturbation series expansion for vibrational nonlinear optical properties. Journal of Chemical Physics, 2002, 116, 5363-5373.	3.0	43
140	Fast O2Binding at Dicopper Complexes Containing Schiff-Base Dinucleating Ligands. Inorganic Chemistry, 2007, 46, 4997-5012.	4.0	43
141	The proton transfer reaction in malonaldehyde derivatives: Substituent effects and quasi-aromaticity of the proton bridge. Chemical Physics, 2007, 342, 43-54.	1.9	43
142	Tuning aromaticity in trigonal alkaline earth metal clusters and their alkali metal salts. Journal of Computational Chemistry, 2009, 30, 2764-2776.	3.3	43
143	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
144	Regiospecific Cï£¿H Bond Activation: Reversible H/D Exchange Promoted by CuI Complexes with Triazamacrocyclic Ligands. Angewandte Chemie - International Edition, 2006, 45, 2941-2944.	13.8	42

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145	New Ru Complexes Containing the N-Tridentate bpea and Phosphine Ligands:Â Consequences of Meridional vs Facial Geometry. Inorganic Chemistry, 2006, 45, 10520-10529.	4.0	41
146	Spin-state splittings of iron(II) complexes with trispyrazolyl ligands. Polyhedron, 2010, 29, 84-93.	2.2	41
147	Molecular mechanism of acid-triggered arylâ€“halide reductive elimination in well-defined arylâ€“CuIIIâ€“halide species. Dalton Transactions, 2010, 39, 10458.	3.3	41
148	Aromaticity Determines the Relative Stability of Kinked vs. Straight Topologies in Polycyclic Aromatic Hydrocarbons. Frontiers in Chemistry, 2018, 6, 561.	3.6	41
149	A Simple Link between Hydrocarbon and Borohydride Chemistries. Chemistry - A European Journal, 2013, 19, 4169-4175.	3.3	40
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