Miquel SolÃ

List of Publications by Year
in descending order

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469 papers	20,593 citations	10351 72 h-index	20307 116 g-index
515 all docs	515 docs citations	515 times ranked	11286 citing authors

#	Article	IF	Citations
1	Initiating Electron Transfer in Doubly Curved Nanographene Upon Supramolecular Complexation of C₆₀. Angewandte Chemie, 2022, 134, .	1.6	9
2	Initiating Electron Transfer in Doubly Curved Nanographene Upon Supramolecular Complexation of C₆₀. Angewandte Chemie - International Edition, 2022, 61, .	7.2	48
3	Effect of Diamine Bridge on Reactivity of Tetradentate ONNO Nickel(II) Complexes. ChemPhysChem, 2022, 23, .	1.0	0
4	Enhancing the Catalytic Performance of Group I, II Metal Halides in the Cycloaddition of CO₂ to Epoxides under Atmospheric Conditions by Cooperation with Homogeneous and Heterogeneous Highly Nucleophilic Aminopyridines: Experimental and Theoretical Study. Journal of Organic Chemistry, 2022, 87, 2873-2886.	1.7	25
5	Path-dependency of energy decomposition analysis & the elusive nature of bonding. Physical Chemistry Chemical Physics, 2022, 24, 2344-2348.	1.3	27
6	Nitrogen-doped molecular bowls as electron donors in photoinduced electron transfer reactions. Nanoscale Advances, 2022, 4, 2180-2188.	2.2	6
7	Aromaticity and Extrusion of Benzenoids Linked to [oâ€COSAN]^{â^'}: Clar Has the Answer. Angewandte Chemie - International Edition, 2022, 61, .	7.2	12
8	Successive Dielsâ€“Alder Cycloadditions of Cyclopentadiene to [10]CPPâŠƒC₆₀: A Computational Study. Journal of Organic Chemistry, 2022, 87, 5149-5157.	1.7	6
9	Highly Selective Synthesis of Seven-Membered Azaspiro Compounds by a Rh(I)-Catalyzed Cycloisomerization/Dielsâ€“Alder Cascade of 1,5-Bisallenes. Journal of Organic Chemistry, 2022, 87, 5279-5286.	1.7	7
10	The importance of the bite angle of metal(III) salen catalysts in the sequestration of CO2 with epoxides in mild conditions. Green Chemical Engineering, 2022, 3, 180-187.	3.3	18
11	KnÃ¶lker Iron Catalysts for Hydrogenation Revisited: A Nonspectator Solvent and Fine-Tuning. Organometallics, 2022, 41, 1204-1215.	1.1	14
12	Three-Dimensional Fully Ï€-Conjugated Macrocycles: When 3D-Aromatic and When 2D-Aromatic-in-3D?. Journal of the American Chemical Society, 2022, 144, 8560-8575.	6.6	28
13	Cageâ€size effects on the encapsulation of <scp> P ₂ </scp> by fullerenes. Journal of Computational Chemistry, 2022, , .	1.5	1
14	The Hunter Falls Prey: Photoinduced Oxidation of C₆₀ in Inclusion Complex with Perfluorocycloparaphenylene. ChemPhysChem, 2022, 23, .	1.0	9
15	Aromaticity of Singlet and Triplet Boron Disk-like Clusters: A Test for Electron Counting Aromaticity Rules. Inorganic Chemistry, 2022, 61, 10116-10125.	1.9	3
16	Aromaticity rules. Nature Chemistry, 2022, 14, 585-590.	6.6	55
17	3D and 2D aromatic units behave like oil and water in the case of benzocarborane derivatives. Nature Communications, 2022, 13, .	5.8	23
18	Mechanistic Studies of Transition-Metal-Catalyzed [2 + 2 + 2] Cycloaddition Reactions. Chemical Reviews, 2021, 121, 1894-1979.	23.0	125

#	Article	IF	Citations
19	Aromaticity of nucleic acid bases. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1509.	6.2	7
20	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.	2.3	50
21	Aromaticity Survival in Hydrofullerenes: The Case of C 66 H 4 with Its Ï€â€Aromatic Circuits. Chemistry - A European Journal, 2021, 27, 802-808.	1.7	9
22	An unprecedented Ï€-electronic circuit involving an odd number of carbon atoms in a grossly warped non-planar nanographene. Chemical Communications, 2021, 57, 3087-3090.	2.2	15
23	Photoinduced electron transfer in nano-Saturn complexes of fullerene. Physical Chemistry Chemical Physics, 2021, 23, 2126-2133.	1.3	8
24	EXCITED-STATE AROMATICITY FOR THE DESIGN OF NEW FUNCTIONAL MATERIALS. , 2021, , .		0
25	Acenes and phenacenes in their lowest-lying triplet states. Does kinked remain more stable than straight?. Physical Chemistry Chemical Physics, 2021, 23, 13574-13582.	1.3	18
26	Photoinduced electron transfer in mechanically interlocked suit[3]ane systems. Journal of Materials Chemistry C, 2021, 9, 9436-9445.	2.7	9
27	The electron density of delocalized bonds (EDDBs) as a measure of local and global aromaticity. , 2021, , 259-284.		11
28	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.	0.5	8
29	Guidelines for Tuning the Excited State HÃ¼ckelâ€“Baird Hybrid Aromatic Character of Proâ€Aromatic Quinoidal Compounds**. Angewandte Chemie, 2021, 133, 10343-10353.	1.6	3
30	Guidelines for Tuning the Excited State HÃ¼ckelâ€“Baird Hybrid Aromatic Character of Proâ€Aromatic Quinoidal Compounds**. Angewandte Chemie - International Edition, 2021, 60, 10255-10265.	7.2	17
31	Efficient synthesis of amine-functionalized graphene oxide by ultrasound-assisted reactions and density functional theory mechanistic insight. Applied Nanoscience (Switzerland), 2021, 11, 1637-1649.	1.6	7
32	How Do Defects in Carbon Nanostructures Regulate the Photoinduced Electron Transfer Processes? The Case of Phenine Nanotubes. ChemPhysChem, 2021, 22, 1178-1186.	1.0	7
33	(Invited) Water-soluble fullerenes (C60 and C70) with photoinduced ROS generation. ECS Meeting Abstracts, 2021, MA2021-01, 618-618.	0.0	0
34	Double-Carrousel Mechanism for Mn-Catalyzed Dehydrogenative Amide Synthesis from Alcohols and Amines. ACS Catalysis, 2021, 11, 6155-6161.	5.5	19
35	Fluxional bis(phenoxy-imine) Zr and Ti catalysts for polymerization. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	2
36	Reactivity of Li+@C60@C240 and Photoinduced Charge Shift in Li+ Doped Giant Nested Fullerenes. ECS Meeting Abstracts, 2021, MA2021-01, 635-635.	0.0	0

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37	[10]CPPâ€Based Inclusion Complexes of Charged Fulleropyrrolidines. Effect of the Charge Location on the Photoinduced Electron Transfer. Chemistry - A European Journal, 2021, 27, 8737-8744.	1.7	10
38	Synthesis of Fused Dihydroazepine Derivatives of Fullerenes by a Rhâ€Catalyzed Cascade Process. Advanced Synthesis and Catalysis, 2021, 363, 3835-3844.	2.1	8
39	Chelation enforcing a dual gold configuration in the catalytic hydroxyphenoxylation of alkynes. Applied Organometallic Chemistry, 2021, 35, e6362.	1.7	5
40	Unexpected Disparity in Photoinduced Reactions of C₆₀ and C₇₀ in Water with the Generation of O₂^{â€¢â€“} or ¹O₂. Jacs Au, 2021, 1, 1601-1611.	3.6	9
41	Predictive Catalysis in Olefin Metathesis with Ruâ€based Catalysts with Annulated C₆₀ Fullerenes in the Nâ€heterocyclic Carbenes. Chemistry - A European Journal, 2021, 27, 18074-18083.	1.7	3
42	Evaluation of charge-transfer rates in fullerene-based donorâ€“acceptor dyads with different density functional approximations. Physical Chemistry Chemical Physics, 2021, 23, 5376-5384.	1.3	18
43	The Relative Stability of Indole Isomers Is a Consequence of the Glidewell-Lloyd Rule. Journal of Physical Chemistry A, 2021, 125, 230-234.	1.1	16
44	Photoinduced electron transfer in non-covalent complexes of C60 and phosphangulene oxide derivatives. Dalton Transactions, 2021, 50, 16214-16222.	1.6	3
45	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.	3.6	5
46	Fast and Simple Evaluation of the Catalysis and Selectivity Induced by External Electric Fields. ACS Catalysis, 2021, 11, 14467-14479.	5.5	14
47	Reactivity of the superhalogen/superalkali ion encapsulating C₆₀ fullerenes. Dalton Transactions, 2021, 51, 203-210.	1.6	2
48	Cyclo[18]carbon: the smallest all-carbon electron acceptor. Chemical Communications, 2020, 56, 352-355.	2.2	78
49	Do Carbon Nanoâ€onions Behave as Nanoscopic Faraday Cages? Aâ€‰Comparison of the Reactivity of C₆₀, C₂₄₀, C₆₀@C₂₄₀, Li⁺@C₆₀, Li⁺@C₂₄₀, and Li⁺@C₆₀@C₂₄₀. Chemistry - A European Journal, 2020, 26, 804-808.	1.7	12
50	The influence of the pH on the reaction mechanism of water oxidation by a Ru(bda) catalyst. Catalysis Today, 2020, 358, 278-283.	2.2	9
51	Iodaneâ€Guided ortho Cî’H Allylation. Angewandte Chemie, 2020, 132, 20376-20382.	1.6	2
52	Bingelâ€“Hirsch Addition of Diethyl Bromomalonate to Ionâ€Encapsulated Fullerenes M@C 60 (M=Ã˜, Li + ,) Tj ETQq0 0 0 rgBT /Overloc	1.7	6
53	Iodaneâ€Guided ortho Cî’H Allylation. Angewandte Chemie - International Edition, 2020, 59, 20201-20207.	7.2	8
54	Probing the Origin of Adaptive Aromaticity in 16â€Valenceâ€Electron Metallapentalenes. Chemistry - A European Journal, 2020, 26, 12902-12902.	1.7	0

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55	Understanding the performance of a bisphosphonate Ru water oxidation catalyst. Dalton Transactions, 2020, 49, 14052-14060.	1.6	10
56	All-metal Baird aromaticity. Chemical Communications, 2020, 56, 12522-12525.	2.2	25
57	Photoinduced electron transfer in nanotubeâŠƒC₇₀ inclusion complexes: phenine vs. nanographene nanotubes. Chemical Communications, 2020, 56, 12624-12627.	2.2	16
58	Electron Transfer in a Li⁺-Doped Zn-Porphyrinâ€"[10]CPPâŠƒFullerene Junction and Charge-Separated Bands with Opposite Response to Polar Environments. Journal of Physical Chemistry B, 2020, 124, 9095-9102.	1.2	16
59	Covalent Functionalization of Single-Walled Carbon Nanotubes by the Bingel Reaction for Building Charge-Transfer Complexes. Journal of Organic Chemistry, 2020, 85, 11721-11731.	1.7	6
60	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.	1.3	12
61	Triquinolineâ€•versus Fullereneâ€Based Cycloparaphenylene Ionic Complexes: Comparison of Photoinduced Chargeâ€Shift Reactions. Chemistry - A European Journal, 2020, 26, 10896-10902.	1.7	10
62	Substituted adenine quartets: interplay between substituent effect, hydrogen bonding, and aromaticity. RSC Advances, 2020, 10, 23350-23358.	1.7	6
63	Mechanism of the Facile Nitrous Oxide Fixation by Homogeneous Ruthenium Hydride Pincer Catalysts. Inorganic Chemistry, 2020, 59, 9374-9383.	1.9	14
64	Probing the Origin of Adaptive Aromaticity in 16â€Valenceâ€Electron Metallapentalenes. Chemistry - A European Journal, 2020, 26, 12964-12971.	1.7	28
65	Effect of Alkali Metal Cations on Length and Strength of Hydrogen Bonds in DNA Base Pairs. ChemPhysChem, 2020, 21, 2112-2126.	1.0	15
66	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.	1.6	7
67	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.	7.2	32
68	Open-Circuit Voltage of Organic Photovoltaics: A Time-Dependent and Unrestricted DFT Study in a P3HT/PCBM Complex. Journal of Physical Chemistry A, 2020, 124, 1300-1305.	1.1	4
69	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
70	(Invited) Reactivity of Li+@C60@C240 and Photoinduced Charge Shift in Li+ Doped Giant Nested Fullerenes. ECS Meeting Abstracts, 2020, MA2020-01, 809-809.	0.0	0
71	(Invited) Preparation of Open-Cage Fullerene Derivatives By Rhodium(I)-Catalyzed [2+2+2] Cycloaddition of Diynes and C60: Synthesis, Computational Studies and Application in Perovskite Solar Cells. ECS Meeting Abstracts, 2020, MA2020-01, 786-786.	0.0	0
72	A Rh-Catalyzed Cycloisomerization/Dielsâ€"Alder Cascade Reaction of 1,5-Bisallenes for the Synthesis of Polycyclic Heterocycles. Organic Letters, 2019, 21, 6608-6613.	2.4	18

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73	Examining the Factors That Govern the Regioselectivity in Rhodium-Catalyzed Alkyne Cyclotrimerization. Organometallics, 2019, 38, 2853-2862.	1.1	34
74	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	1.5	113
75	Special Collection: Computational Chemistry. ChemistryOpen, 2019, 8, 814-816.	0.9	3
76	Mechanism of the Manganese-Pincer-Catalyzed Acceptorless Dehydrogenative Coupling of Nitriles and Alcohols. Journal of the American Chemical Society, 2019, 141, 2398-2403.	6.6	69
77	Hypsochromic solvent shift of the charge separation band in ionic donorâ€“acceptor Li⁺@C₆₀âŠ‚[10]CPP. Chemical Communications, 2019, 55, 11195-11198.	2.2	23
78	Exploiting the Aromatic Chameleon Character of Fulvenes for Computational Design of Bairdâ€Aromatic Triplet Ground State Compounds. Chemistry - an Asian Journal, 2019, 14, 1870-1878.	1.7	13
79	Regioselectivity in Dielsâ€“Alder Cycloadditions of #6094C68 Fullerene with a Triplet Ground State. Journal of Organic Chemistry, 2019, 84, 9017-9024.	1.7	7
80	Photoinduced Charge Shift in Li⁺-Doped Giant Nested Fullerenes. Journal of Physical Chemistry C, 2019, 123, 16525-16532.	1.5	13
81	Effect of Exocyclic Substituents and Ï€-System Length on the Electronic Structure of Chichibabin Diradical(oid)s. ACS Omega, 2019, 4, 10845-10853.	1.6	10
82	InnenrÃ¼cktitelbild: Allâ€Fullerene Electron Donorâ€“Acceptor Conjugates (Angew. Chem. 21/2019). Angewandte Chemie, 2019, 131, 7217-7217.	1.6	1
83	Allâ€Fullerene Electron Donorâ€“Acceptor Conjugates. Angewandte Chemie - International Edition, 2019, 58, 6932-6937.	7.2	35
84	Is Excitedâ€State Aromaticity a Driving Force for Planarization of Dibenzannelated 8Ï€â€Electron Heterocycles?. ChemPlusChem, 2019, 84, 712-721.	1.3	38
85	Allâ€Fullerene Electron Donorâ€“Acceptor Conjugates. Angewandte Chemie, 2019, 131, 7006-7011.	1.6	13
86	Electron Delocalization in Planar Metallacycles: HÃ¼ckel or MÃ¶bius Aromatic?. ChemistryOpen, 2019, 8, 219-227.	0.9	49
87	The Coulomb Hole of the Ne Atom. ChemistryOpen, 2019, 8, 411-417.	0.9	6
88	Open-shell jellium aromaticity in metal clusters. Chemical Communications, 2019, 55, 5559-5562.	2.2	15
89	Decomposition of the electronic activity in competing [5,6] and [6,6] cycloaddition reactions between C₆₀ and cyclopentadiene. Physical Chemistry Chemical Physics, 2019, 21, 5039-5048.	1.3	11
90	Photoinduced electron transfer and unusual environmental effects in fullereneâ€“Zn-porphyrinâ€“BODIPY triads. Physical Chemistry Chemical Physics, 2019, 21, 25098-25107.	1.3	22

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91	Tuning the Strength of the Resonance-Assisted Hydrogen Bond in Acenes and Phenacenes with Two o-Hydroxyaldehyde Groupsâ€"The Importance of Topology. Journal of Organic Chemistry, 2019, 84, 15538-15548.	1.7	13
92	Connecting and combining rules of aromaticity. Towards a unified theory of aromaticity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1404.	6.2	37
93	Peculiar Photoinduced Electron Transfer in Porphyrinâ€"Fullerene Akamptisomers. Chemistry - A European Journal, 2019, 25, 2577-2585.	1.7	9
94	(Invited) Photoinduced Charge Separation in Several Dyads Involving Fullerenes. ECS Meeting Abstracts, 2019, , .	0.0	0
95	52 GAMES WITH THE PERIODIC TABLE AND BEYOND. , 2019, , .		0
96	Rationalizing the Regioselectivity of the Dielsâ€"Alder Biscycloaddition of Fullerenes. Journal of Organic Chemistry, 2018, 83, 3285-3292.	1.7	11
97	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. Chemistry - A European Journal, 2018, 24, 9853-9859.	1.7	28
98	Reliable charge assessment on encapsulated fragment for endohedral systems. Scientific Reports, 2018, 8, 2882.	1.6	5
99	Tuning the Strength of the Resonance-Assisted Hydrogen Bond in o-Hydroxybenzaldehyde by Substitution in the Aromatic Ring¹. Journal of Physical Chemistry A, 2018, 122, 2279-2287.	1.1	28
100	On the regioselectivity of the Dielsâ€"Alder cycloaddition to C₆₀ in high spin states. Physical Chemistry Chemical Physics, 2018, 20, 11577-11585.	1.3	10
101	Electron-Pair Distribution in Chemical Bond Formation. Journal of Physical Chemistry A, 2018, 122, 1916-1923.	1.1	6
102	Aromaticity of acenes: the model of migrating Ï€-circuits. Physical Chemistry Chemical Physics, 2018, 20, 13430-13436.	1.3	36
103	Mechanism of the Selective Fe-Catalyzed Arene Carbonâ€"Hydrogen Bond Functionalization. ACS Catalysis, 2018, 8, 4313-4322.	5.5	32
104	Influence of the charge on the reactivity of azafullerenes. Physical Chemistry Chemical Physics, 2018, 20, 28011-28018.	1.3	11
105	Aromaticity Determines the Relative Stability of Kinked vs. Straight Topologies in Polycyclic Aromatic Hydrocarbons. Frontiers in Chemistry, 2018, 6, 561.	1.8	41
106	Stereocontrolled Photoinduced Electron Transfer in Metalâ€Fullerene Hybrids. Chemistry - A European Journal, 2018, 24, 13020-13025.	1.7	17
107	Regioselectivity of the Pausonâ€"Khand reaction in single-walled carbon nanotubes. Nanoscale, 2018, 10, 15078-15089.	2.8	11
108	Expeditious Preparation of Open-Cage Fullerenes by Rhodium(I)-Catalyzed [2+2+2] Cycloaddition of Diynes and C60 : Anâ€‰Experimental and Theoretical Study. Chemistry - A European Journal, 2018, 24, 10561-10561.	1.7	0

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109	Quantum Mechanics/Molecular Mechanics Studies on the Relative Reactivities of Compound I and II in Cytochrome P450 Enzymes. International Journal of Molecular Sciences, 2018, 19, 1974.	1.8	14
110	The electronic structure and stability of germanium tubes Ge₃₀H₁₂ and Ge₃₃H₁₂. Physical Chemistry Chemical Physics, 2018, 20, 23467-23479.	1.3	6
111	Expeditious Preparation of Openâ€Cage Fullerenes by Rhodium(I)â€Catalyzed [2+2+2] Cycloaddition of Diynes and C₆₀: Anâ€‰Experimental and Theoretical Study. Chemistry - A European Journal, 2018, 24, 10653-10661.	1.7	28
112	Tuning diastereoisomerism in platinum(ii) phosphino- and aminothiolato hydrido complexes. New Journal of Chemistry, 2017, 41, 3015-3028.	1.4	1
113	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.	1.7	71
114	Is coronene better described by <scp>C</scp>lar's aromatic Ï€â€sextet model or by the AdNDP representation?. Journal of Computational Chemistry, 2017, 38, 1606-1611.	1.5	30
115	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.	1.5	69
116	Understanding the Reactivity of Ionâ€Encapsulated Fullerenes. Chemistry - A European Journal, 2017, 23, 11030-11036.	1.7	33
117	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.	1.7	55
118	Mechanism of the Suzukiâ€“Miyaura Cross-Coupling Reaction Mediated by [Pd(NHC)(allyl)Cl] Precatalysts. Organometallics, 2017, 36, 2088-2095.	1.1	68
119	Rationalizing the relative abundances of trimetallic nitride template-based endohedral metallofullerenes from aromaticity measures. Chemical Communications, 2017, 53, 4140-4143.	2.2	5
120	Predicting and Understanding the Reactivity of Aza[60]fullerenes. Journal of Organic Chemistry, 2017, 82, 754-758.	1.7	20
121	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.	1.4	9
122	The electron density of delocalized bonds (EDDB) applied for quantifying aromaticity. Physical Chemistry Chemical Physics, 2017, 19, 28970-28981.	1.3	114
123	A Computational Study of the Intermolecular [2+2+2] Cycloaddition of Acetylene and C₆₀ Catalyzed by Wilkinson's Catalyst. Chemistry - A European Journal, 2017, 23, 15067-15072.	1.7	11
124	Does the endohedral borospherene supersalt FLi₂@B₃₉maintain the â€œsuperâ€• properties of its subunits?. Physical Chemistry Chemical Physics, 2017, 19, 21276-21281.	1.3	6
125	The key role of aromaticity in the structure and reactivity of C60 and endohedral metallofullerenes. Inorganica Chimica Acta, 2017, 468, 38-48.	1.2	8
126	Rhodiumâ€Catalyzed [2+2+2] Cycloaddition Reactions of Linear Alleneâ€“Eneâ€“Ynes to afford Fused Tricyclic Scaffolds: Insights into the Mechanism. Chemistry - A European Journal, 2017, 23, 14889-14899.	1.7	22

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127	Unusual reactivity of rhodium carbenes with allenes: an efficient asymmetric synthesis of methylenetetrahydropyran scaffolds. Chemical Communications, 2017, 53, 9922-9925.	2.2	15
128	Effect of incarcerated HF on the exohedral chemical reactivity of HF@C₆₀. Chemical Communications, 2017, 53, 10993-10996.	2.2	26
129	Why Aromaticity Is a Suspicious Concept? Why?. Frontiers in Chemistry, 2017, 5, 22.	1.8	108
130	Theoretical estimation of the rate of photoinduced charge transfer reactions in triphenylamine C₆₀ donorâ€“acceptor conjugate. Journal of Computational Chemistry, 2016, 37, 1396-1405.	1.5	10
131	Reactivity and Selectivity of Bowlâ€Shaped Polycyclic Aromatic Hydrocarbons: Relationship to C₆₀. Chemistry - A European Journal, 2016, 22, 1368-1378.	1.7	31
132	In Silico Olefin Metathesis with Ruâ€Based Catalysts Containing Nâ€Heterocyclic Carbenes Bearing C₆₀ Fullerenes. Chemistry - A European Journal, 2016, 22, 6617-6623.	1.7	15
133	Understanding the Reactivity of Planar Polycyclic Aromatic Hydrocarbons: Towards the Graphene Limit. Chemistry - A European Journal, 2016, 22, 10572-10580.	1.7	27
134	Photoinduced Charge Separation in the Carbon Nano-Onion C₆₀@C₂₄₀. Journal of Physical Chemistry A, 2016, 120, 5798-5804.	1.1	10
135	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.	1.7	23
136	The Regioselectivity of Bingelâ€“Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie, 2016, 128, 2420-2423.	1.6	9
137	Celebrating the 150th anniversary of the KekulÃ© benzene structure. Physical Chemistry Chemical Physics, 2016, 18, 11587-11588.	1.3	26
138	Rules of Aromaticity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 321-335.	0.6	7
139	Structural Preferences in Phosphanylthiolato Platinum(II) Complexes. ChemistryOpen, 2016, 5, 51-59.	0.9	6
140	Planar vs. three-dimensional X₆^{2â^'}, X₂Y₄^{2â^'}, and X₃Y₃^{2â^'} (X, Y = B,) Tj ETQq0 0 0 rgBT /Ov Physical Chemistry Chemical Physics, 2016, 18, 21102-21110.	1.3	7
141	The Driving Force of Photoinduced Charge Separation in Metalâ€Clusterâ€Encapsulated Triphenylamineâ€[80]fullerenes. Chemistry - A European Journal, 2016, 22, 17305-17310.	1.7	5
142	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.	0.5	24
143	The Regioselectivity of Bingelâ€“Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie - International Edition, 2016, 55, 2374-2377.	7.2	37
144	Analysis of a Compound Class with Triplet States Stabilized by Potentially Baird Aromatic [10]Annulenyl Dicationic Rings. Chemistry - A European Journal, 2016, 22, 2793-2800.	1.7	30

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145	HÃ¼ckel's Rule of Aromaticity Categorizes Aromatic closo Boron Hydride Clusters. Chemistry - A European Journal, 2016, 22, 7437-7443.	1.7	103
146	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.	1.5	10
147	Fmocâ€“RGDS based fibrils: atomistic details of their hierarchical assembly. Physical Chemistry Chemical Physics, 2016, 18, 1265-1278.	1.3	17
148	Octahedral aromaticity in ^{2S+1}A_{1g} X₆^q clusters (X =) Tj ETQq0 0 0 rgBT /Overlock	1.3	12
149	Bonding description of the Harpoon mechanism. Molecular Physics, 2016, 114, 1345-1355.	0.8	13
150	Structural Preferences in Phosphanylthiolato Platinum(II) Complexes. ChemistryOpen, 2016, 5, 2-2.	0.9	1
151	(4 + 2) and (2 + 2) Cycloadditions of Benzyne to C₆₀ and Zig-Zag Single-Walled Carbon Nanotubes: The Effect of the Curvature. Journal of Physical Chemistry C, 2016, 120, 1716-1726.	1.5	34
152	Nitrite to nitric oxide interconversion by heme FeII complex assisted by [CuI(tmpa)]+. Structural Chemistry, 2016, 27, 409-417.	1.0	3
153	(Invited) The Regioselectivity of the Diels-Alder and Bingel-Hirsch Additions to La@C2v -C82. ECS Meeting Abstracts, 2016, , .	0.0	0
154	(Invited) Photoinduced Charge Transfer Reactions and Excited State Properties in Triphenylamine C60 Donor-Acceptor Conjugates. ECS Meeting Abstracts, 2016, , .	0.0	0
155	(Invited) Aromaticity, Cage Structure, and Relative Abundancy of Endohedral Metallofullerenes. ECS Meeting Abstracts, 2016, , .	0.0	0
156	(Invited) The Regioselectivity of Bingel-Hirsch Cycloadditions on IPR Endohedral Metallofullerenes. ECS Meeting Abstracts, 2016, , .	0.0	0
157	Enantioselective Rhodium(I) Donor Carbenoidâ€Mediated Cascade Triggered by a Baseâ€Free Decomposition of Arylsulfonyl Hydrazones. Chemistry - A European Journal, 2015, 21, 16240-16245.	1.7	37
158	On the Reaction Mechanism of the Rhodium-Catalyzed Arylation of Fullerene (C₆₀) with Organoboron Compounds in the Presence of Water. ChemistryOpen, 2015, 4, 774-778.	0.9	12
159	Enantiospecific cisâ€“trans Isomerization in Chiral Fulleropyrrolidines: Hydrogen-Bonding Assistance in the Carbanion Stabilization in H₂O@C₆₀. Journal of the American Chemical Society, 2015, 137, 1190-1197.	6.6	40
160	Extent of charge separation and exciton delocalization for electronically excited states in a triphenylamine-C60 donorâ€“acceptor conjugate: a combined molecular dynamics and TD-DFT study. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	13
161	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.	2.3	65
162	Three-center bonding analyzed from correlated and uncorrelated third-order reduced density matrices. Computational and Theoretical Chemistry, 2015, 1053, 173-179.	1.1	8

#	Article	IF	Citations
163	On the existence and characterization of molecular electrides. Chemical Communications, 2015, 51, 4865-4868.	2.2	68
164	Understanding the Reactivity of Endohedral Metallofullerenes: C₇₈ versus Sc₃N@C₇₈. Chemistry - A European Journal, 2015, 21, 5760-5768.	1.7	45
165	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.	1.9	46
166	Why 1,2-quinone derivatives are more stable than their 2,3-analogues?. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	16
167	Quantifying aromaticity with electron delocalisation measures. Chemical Society Reviews, 2015, 44, 6434-6451.	18.7	335
168	Computational Insight into the Mechanism of Alkane Hydroxylation by Non-heme Fe(PyTACN) Iron Complexes. Effects of the Substrate and Solvent. Inorganic Chemistry, 2015, 54, 8223-8236.	1.9	24
169	Reusable manganese compounds containing pyrazole-based ligands for olefin epoxidation reactions. Dalton Transactions, 2015, 44, 17529-17543.	1.6	18
170	A theoretical study of the aromaticity in neutral and anionic borole compounds. Dalton Transactions, 2015, 44, 6740-6747.	1.6	37
171	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	1.1	99
172	Understanding the Exohedral Functionalization of Endohedral Metallofullerenes Metallofullerenes. Carbon Materials, 2015, , 67-99.	0.2	0
173	Computational insight into Wilkinson's complex catalyzed [2Â+Â2Â+Â2] cycloaddition mechanism leading to pyridine formation. Journal of Organometallic Chemistry, 2014, 768, 15-22.	0.8	15
174	Exploring the Potential Energy Surface of E₂P₄ Clusters (E=Groupâ€…13 Element): The Quest for Inverse Carbonâ€Free Sandwiches. Chemistry - A European Journal, 2014, 20, 4583-4590.	1.7	19
175	Stereoselective Rhodiumâ€Catalysed [2+2+2] Cycloaddition of Linear Alleneâ€“Ene/Yneâ€“Allene Substrates: Reactivity and Theoretical Mechanistic Studies. Chemistry - A European Journal, 2014, 20, 5034-5045.	1.7	37
176	Origin of Reactivity Trends of Noble Gas Endohedral Fullerenes Ng₂@C₆₀ (Ng) Tj ETQq0 0 0 rgBT /Overlock 10	2.3	34
177	A new mild synthetic route to N-arylated pyridazinones from aryldiazonium salts. Chemical Communications, 2014, 50, 8073-8076.	2.2	6
178	Ï€â€…Aromaticity and Threeâ€Dimensional Aromaticity: Two sides of the Same Coin?. Angewandte Chemie - International Edition, 2014, 53, 12191-12195.	7.2	242
179	Reaction Mechanisms for the Formation of Mono- And Dipropylene Glycol from the Propylene Oxide Hydrolysis over ZSM-5 Zeolite. Journal of Physical Chemistry C, 2014, 118, 21952-21962.	1.5	15
180	The role of aromaticity in determining the molecular structure and reactivity of (endohedral) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 62 Td	18.7	97

#	Article	IF	Citations
181	Electroactive polymers for the detection of morphine. Journal of Polymer Research, 2014, 21, 1.	1.2	6
182	Aromaticity and Magnetic Properties of 1â€•and 2â€Indenones and Their Aza Derivatives. European Journal of Organic Chemistry, 2014, 2014, 5370-5377.	1.2	9
183	Analysis of the Aromaticity of Five-Membered Heterometallacycles Containing Os, Ru, Rh, and Ir. Organometallics, 2014, 33, 1762-1773.	1.1	31
184	New Approximation to the Third-Order Density. Application to the Calculation of Correlated Multicenter Indices. Journal of Chemical Theory and Computation, 2014, 10, 3055-3065.	2.3	31
185	Dinuclear Ruâ€“Aqua Complexes for Selective Epoxidation Catalysis Based on Supramolecular Substrate Orientation Effects. Chemistry - A European Journal, 2014, 20, 3898-3902.	1.7	32
186	Aromatic properties of 8-hydroxyquinoline and its metal complexes. Open Chemistry, 2013, 11, 655-663.	1.0	8
187	Aromaticity as the driving force for the stability of non-IPR endohedral metallofullerene Bingelâ€“Hirsch adducts. Chemical Communications, 2013, 49, 8767.	2.2	21
188	Maximum Aromaticity as a Guiding Principle for the Most Suitable Hosting Cages in Endohedral Metallofullerenes. Angewandte Chemie - International Edition, 2013, 52, 9275-9278.	7.2	55
189	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.	1.1	9
190	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.	1.1	13
191	Simple and cheap steric and electronic characterization of the reactivity of Ru(II) complexes containing oxazoline ligands as epoxidation catalysts. Chemical Physics Letters, 2013, 577, 142-146.	1.2	6
192	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.	1.9	16
193	A Complete Guide on the Influence of Metal Clusters in the Dielsâ€“Alder Regioselectivity of I_hâ€“C₈₀ Endohedral Metallofullerenes. Chemistry - A European Journal, 2013, 19, 14931-14940.	1.7	37
194	Analysis of the Relative Stabilities of Ortho, Meta, and Para MClY(XC₄H₄)(PH₃)₂ Heterometallabenzenes (M = Rh,) Tj ETQq1 0 0 rgBT/Overloc	1.1	36
195	Examining the formation of specific interactions between poly(3,4-ethylenedioxythiophene) and nucleotide bases. RSC Advances, 2013, 3, 2639.	1.7	7
196	Electrochemical control of the regioselectivity in the exohedral functionalization of C60: the role of aromaticity. Chemical Communications, 2013, 49, 1220.	2.2	44
197	Metalloaromaticity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 105-122.	6.2	105
198	Dielsâ€“Alder and Retroâ€Dielsâ€“Alder Cycloadditions of (1,2,3,4,5â€Pentamethyl)cyclopentadiene to La@C₂vâ€“C₈₂: Regioselectivity and Product Stability. Chemistry - A European Journal, 2013, 19, 4468-4479.	1.7	27

#	Article	IF	Citations
199	A Simple Link between Hydrocarbon and Borohydride Chemistries. Chemistry - A European Journal, 2013, 19, 4169-4175.	1.7	40
200	Why Do Cycloaddition Reactions Involving C₆₀ Prefer [6,6] over [5,6] Bonds?. Chemistry - A European Journal, 2013, 19, 7416-7422.	1.7	100
201	Ruthenium Complexes with Chiral Bis-Pinene Ligands: an Array of Subtle Structural Diversity. Inorganic Chemistry, 2013, 52, 4985-4992.	1.9	7
202	Nuclear magnetic resonance shieldings of water clusters: is it possible to reach the complete basis set limit by extrapolation?. Molecular Physics, 2013, 111, 1332-1344.	0.8	5
203	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.	1.1	152
204	A Full Dimensionality Approach to Evaluate the Nonlinear Optical Properties of Molecules with Large Amplitude Anharmonic Tunneling Motions. Journal of Chemical Theory and Computation, 2013, 9, 520-532.	2.3	9
205	Nâ€Tetradentate SPANamine Derivatives and Their Mn^{II}â€Complexes as Catalysts for Epoxidation of Alkenes. European Journal of Inorganic Chemistry, 2013, 2013, 1213-1224.	1.0	19
206	Forty years of Clar's aromatic Ï€-sextet rule. Frontiers in Chemistry, 2013, 1, 22.	1.8	332
207	Complete Ïƒ* intramolecular aromatic hydroxylation mechanism through O2 activation by a Schiff base macrocyclic dicopper(I) complex. Beilstein Journal of Organic Chemistry, 2013, 9, 585-593.	1.3	6
208	Tuning the Electronic Properties by Width and Length Modifications of Narrow- Diameter Carbon Nanotubes for Nanomedicine. Current Medicinal Chemistry, 2012, 19, 5219-5225.	1.2	17
209	A new DFT functional based on spin-states and SN2 barriers. , 2012, , .		0
210	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.	1.3	18
211	On the electronic structure of second generation Hoveydaâ€"Grubbs alkene metathesis precursors. Computational and Theoretical Chemistry, 2012, 996, 57-67.	1.1	21
212	Product formation in the Prato reaction on Sc3N@D5h-C80: preference for [5,6]-bonds, and not pyracylenic bonds. Chemical Communications, 2012, 48, 2486.	2.2	26
213	Properties of poly(3-halidethiophene)s. Physical Chemistry Chemical Physics, 2012, 14, 10050.	1.3	8
214	The Frozen Cage Model: A Computationally Low-Cost Tool for Predicting the Exohedral Regioselectivity of Cycloaddition Reactions Involving Endohedral Metallofullerenes. Journal of Chemical Theory and Computation, 2012, 8, 1671-1683.	2.3	18
215	Direct Detection of Key Intermediates in Rhodium(I)â€Catalyzed [2+2+2] Cycloadditions of Alkynes by ESIâ€MS. Chemistry - A European Journal, 2012, 18, 13097-13107.	1.7	37
216	The linear response kernel of conceptual DFT as a measure of aromaticity. Physical Chemistry Chemical Physics, 2012, 14, 3960.	1.3	51

#	Article	IF	Citations
217	Electronic and Vibrational Nonlinear Optical Properties of Five Representative Electrides. Journal of Chemical Theory and Computation, 2012, 8, 2688-2697.	2.3	78
218	On the reliability of the maximum hardness and minimum polarizability principles in nontotally symmetric vibrations. , 2012, , .		1
219	The Exohedral Dielsâ€“Alder Reactivity of the Titanium Carbide Endohedral Metallofullerene Ti₂C₂@D₃h</sub>â€C₇₈: Comparison with D₃h</sub>â€C₇₈ and M₃N@D₃h</sub>â€C₇₈ (M=Sc and Y) Reactivity. Chemistry - A	1.7	54
220	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.	1.7	49
221	Open-shell spherical aromaticity: the 2N2 + 2N + 1 (with S = N + Â½) rule. Chemical Communications, 2011, 47, 11647.	2.2	49
222	A donor-functionalized, silyl-substituted pentadienyllithium: structural insight from experiment and theory. Chemical Communications, 2011, 47, 6162.	2.2	14
223	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2011, 7, 1231-1231.	2.3	7
224	Nuclear Shieldings with the SSB-D Functional. Journal of Physical Chemistry A, 2011, 115, 1250-1256.	1.1	16
225	RhCl(PPh₃)₃-Catalyzed Intramolecular Cycloaddition of Enediynes: The Nature of the Tether and Substituents Controls the Reaction Mechanism. Organometallics, 2011, 30, 3151-3159.	1.1	22
226	New Ru(II) Complexes Containing Oxazoline Ligands As Epoxidation Catalysts. Influence of the Substituents on the Catalytic Performance. Inorganic Chemistry, 2011, 50, 6044-6054.	1.9	30
227	All-metal aromatic clusters M42â^' (M = B, Al, and Ga). Are Ï€-electrons distortive or not?. Physical Chemistry Chemical Physics, 2011, 13, 20673.	1.3	14
228	DFT Study of Thermal 1,3-Dipolar Cycloaddition Reactions between Alkynyl Metal(0) Fischer Carbene Complexes and 3H-1,2-Dithiole-3-thione Derivatives. Organometallics, 2011, 30, 466-476.	1.1	38
229	Understanding Conjugation and Hyperconjugation from Electronic Delocalization Measures. Journal of Physical Chemistry A, 2011, 115, 13104-13113.	1.1	30
230	The reactivity of endohedral fullerenes. What can be learnt from computational studies?. Physical Chemistry Chemical Physics, 2011, 13, 3585-3603.	1.3	128
231	Routes of Ï€-Electron Delocalization in 4-Substituted-1,2-benzoquinones. Journal of Organic Chemistry, 2011, 76, 550-556.	1.7	15
232	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.	1.7	43
233	Dispersion Corrections Essential for the Study of Chemical Reactivity in Fullerenes. Journal of Physical Chemistry A, 2011, 115, 3491-3496.	1.1	117
234	Binding of 6-mer single-stranded homo-nucleotides to poly(3,4-ethylenedioxythiophene): specific hydrogen bonds with guanine. Soft Matter, 2011, 7, 9922.	1.2	13

#	Article	IF	Citations
235	Organomagnesium clusters: Structure, stability, and bonding in archetypal models. Journal of Organometallic Chemistry, 2011, 696, 4104-4111.	0.8	13
236	Ab Initio Design of Chelating Ligands Relevant to Alzheimerâ€™s Disease: Influence of Metalloaromaticity. Journal of Physical Chemistry A, 2011, 115, 12659-12666.	1.1	20
237	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.	1.1	46
238	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.	6.6	232
239	Editorial [Hot Topic: Electron Delocalization in Organic Chemistry (Guest Editors: Dr. Eduard Matito) Tj ETQq1 1 0.784314 rgBT /Over	0.9	0
240	Electron delocalization and aromaticity in low-lying excited states of archetypal organic compounds. Physical Chemistry Chemical Physics, 2011, 13, 20690.	1.3	116
241	A multi-scale approach to spin crossover in Fe(ii) compounds. Physical Chemistry Chemical Physics, 2011, 13, 10449.	1.3	19
242	Aromaticity and electronic delocalization in all-metal clusters with single, double, and triple aromatic character. Theoretical Chemistry Accounts, 2011, 128, 419-431.	0.5	57
243	Measuring electron sharing between atoms in first-principle simulations. Theoretical Chemistry Accounts, 2011, 130, 27-36.	0.5	6
244	Theoretical studies on aromaticity of selected hydroxypyrones. Part 3#. Chelatoaromaticity phenomenon in metalcomplexes of hydroxypyrones. Journal of Physical Organic Chemistry, 2011, 24, 499-506.	0.9	16
245	Performance of 3Dâ€spaceâ€based atomsâ€inâ€molecules methods for electronic delocalization aromaticity indices. Journal of Computational Chemistry, 2011, 32, 386-395.	1.5	36
246	Interâ€•and intramolecular dispersion interactions. Journal of Computational Chemistry, 2011, 32, 1117-1127.	1.5	34
247	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.	1.5	61
248	Intramolecular [2+2+2] Cycloaddition Reactions of Yneâ€•eneâ€•yne and Yneâ€•yneâ€•ene Enediynes Catalysed by Rh^I: Experimental and Theoretical Mechanistic Studies. Chemistry - A European Journal, 2011, 17, 14493-14507.	1.7	32
249	The Chemical Reactivity of Fullerenes and Endohedral Fullerenes: A Theoretical Perspective. Carbon Materials, 2011, , 57-78.	0.2	2
250	An account on multicenter bonding and its relationship with aromaticity. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C85-C85.	0.3	0
251	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.	1.3	38
252	On the Mechanism of Action of Fullerene Derivatives in Superoxide Dismutation. Chemistry - A European Journal, 2010, 16, 3207-3214.	1.7	49

#	Article	IF	Citations
253	Reactivity and Regioselectivity of Noble Gas Endohedral Fullerenes Ng@C60 and Ng2@C60 (Ng=He-Xe). Chemistry - A European Journal, 2010, 16, 3878-3878.	1.7	6
254	Spin-state splittings of iron(II) complexes with trispyrazolyl ligands. Polyhedron, 2010, 29, 84-93.	1.0	41
255	A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity. Symmetry, 2010, 2, 1156-1179.	1.1	115
256	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.	2.3	84
257	Computational methods to predict the reactivity of nanoparticles through structureâ€“property relationships. Expert Opinion on Drug Delivery, 2010, 7, 295-305.	2.4	64
258	Mechanism of the Aminolysis of Fischer Alkoxy and Thiocarbene Complexes: A DFT Study. Journal of Organic Chemistry, 2010, 75, 5821-5836.	1.7	19
259	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2010, 6, 2736-2742.	2.3	115
260	Density Functional Study of the [2+2+2] Cyclotrimerization of Acetylene Catalyzed by Wilkinsonâ€™s Catalyst, RhCl(PPh₃)₃. Organometallics, 2010, 29, 562-569.	1.1	68
261	Density Functional Calculations of E2 and S_N2 Reactions: Effects of the Choice of Method, Algorithm, and Numerical Accuracy. Journal of Chemical Theory and Computation, 2010, 6, 3145-3152.	2.3	33
262	Influence of Confinement on Hydrogen Bond Energy. The Case of the FHÂ·Â·Â·NCH Dimer. Journal of Physical Chemistry A, 2010, 114, 10253-10260.	1.1	31
263	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.	6.6	131
264	Reaction Mechanisms for Graphene and Carbon Nanotube Fluorination. Journal of Physical Chemistry C, 2010, 114, 3340-3345.	1.5	56
265	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.	1.1	38
266	Spin-State-Corrected Gaussian-Type Orbital Basis Sets. Journal of Physical Chemistry A, 2010, 114, 7191-7197.	1.1	47
267	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.	2.3	81
268	Molecular mechanism of acid-triggered arylâ€“halide reductive elimination in well-defined arylâ€“CuIIIâ€“halide species. Dalton Transactions, 2010, 39, 10458.	1.6	41
269	Ene reactions between two alkynes? Doors open to thermally induced cycloisomerization of macrocyclic triynes and enediynes. Chemical Communications, 2010, 46, 2944.	2.2	23
270	A new all-round density functional based on spin states and S[sub N]2 barriers. Journal of Chemical Physics, 2009, 131, 094103.	1.2	113

#	Article	IF	Citations
271	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.	1.7	49
272	Reactivity and Regioselectivity of Noble Gas Endohedral Fullerenes Ng@C₆₀ and Ng₂@C₆₀ (Ng=Heâ€“Xe). Chemistry - A European Journal, 2009, 15, 13111-13123.	1.7	45
273	DÃ¶tz Benzannulation Reactions: Heteroatom and Substituent Effects in Chromium Fischer Carbene Complexes. Chemistry - A European Journal, 2009, 15, 12503-12520.	1.7	21
274	Homolytic versus Heterolytic Dissociation of Alkalimetal Halides: The Effect of Microsolvation. ChemPhysChem, 2009, 10, 2955-2965.	1.0	14
275	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.	1.0	15
276	On the Regioselective Intramolecular Nucleophilic Addition of Thiols to C₆₀. European Journal of Organic Chemistry, 2009, 2009, 6231-6238.	1.2	16
277	Modeling the structureâ€property relationships of nanoneedles: A journey toward nanomedicine. Journal of Computational Chemistry, 2009, 30, 275-284.	1.5	76
278	Tuning aromaticity in trigonal alkaline earth metal clusters and their alkali metal salts. Journal of Computational Chemistry, 2009, 30, 2764-2776.	1.5	43
279	Theoretical study of the hydroxylation of phenolates by the Cu2O2(N,Nâ€²-dimethylethylenediamine)2 2+ complex. Journal of Biological Inorganic Chemistry, 2009, 14, 229-242.	1.1	17
280	Theoretical study of the hydroxylation of phenols mediated by an end-on bound superoxoâ€“copper(II) complex. Journal of Biological Inorganic Chemistry, 2009, 14, 273-285.	1.1	12
281	Excess charge delocalization in organic and biological molecules: some theoretical notions. Theoretical Chemistry Accounts, 2009, 123, 29-40.	0.5	9
282	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.	9.5	141
283	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.	1.1	63
284	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.	6.6	76
285	Structure, Bonding, and Relative Stability of the Ground and Low-Lying Electronic States of CuO2. The Role of Exact Exchange. Journal of Physical Chemistry A, 2009, 113, 1308-1317.	1.1	19
286	Interplay between Intramolecular Resonance-Assisted Hydrogen Bonding and Local Aromaticity. II. 1,3-Dihydroxyaryl-2-aldehydes. Journal of Organic Chemistry, 2009, 74, 2059-2066.	1.7	68
287	H-Bond-Assisted Regioselective (cis-1) Intramolecular Nucleophilic Addition of the Hydroxyl Group to [60]Fullerene. Journal of Organic Chemistry, 2009, 74, 1480-1487.	1.7	37
288	Competitive Retro-Cycloaddition Reaction in Fullerene Dimers Connected through Pyrrolidinopyrazolino Rings. Journal of Organic Chemistry, 2009, 74, 8174-8180.	1.7	25

#	Article	IF	Citations
289	Regioselective Intramolecular Nucleophilic Addition of Alcohols to C₆₀: One-Step Formation of acis-1 Bicyclic-Fused Fullerene. Journal of Organic Chemistry, 2009, 74, 6253-6259.	1.7	33
290	Local Aromaticity of Pristine and Fluorinated Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2009, 9, 6078-6083.	0.9	8
291	Aromaticity and Chemical Reactivity. , 2009, , .		5
292	On the Mechanism of the Thermal Retrocycloaddition of Pyrrolidinofullerenes (Retroâ€Prato) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 622	1.7	56
293	The hardness kernel as the basis for global and local reactivity indices. Journal of Computational Chemistry, 2008, 29, 1064-1072.	1.5	34
294	On the performance of some aromaticity indices: A critical assessment using a test set. Journal of Computational Chemistry, 2008, 29, 1543-1554.	1.5	261
295	Mechanistic theoretical insight of Ru(II) catalysts with a meridionalâ€“facial bpea fashion competition. Chemical Physics Letters, 2008, 458, 200-204.	1.2	10
296	Coordination of bis(tricarbonylchromium) complexes to small polycyclic aromatic hydrocarbons: Structure, relative stabilities, and bonding. Chemical Physics Letters, 2008, 465, 181-189.	1.2	7
297	Nanosized trigonal prismatic and antiprismatic CuII coordination cages based on tricarboxylate linkers. Dalton Transactions, 2008, , 1679.	1.6	15
298	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.	2.3	86
299	Analysis of HÃ¼ckelâ€™s [4n+ 2] Rule through Electronic Delocalization Measures. Journal of Physical Chemistry A, 2008, 112, 13231-13238.	1.1	38
300	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.	6.6	62
301	Importance of the Basis Set for the Spin-State Energetics of Iron Complexes. Journal of Physical Chemistry A, 2008, 112, 6384-6391.	1.1	131
302	New Ruthenium(II) Complexes with Enantiomerically Pure Bis- and Tris(pinene)-Fused Tridentate Ligands. Synthesis, Characterization and Stereoisomeric Analysis. Inorganic Chemistry, 2008, 47, 8016-8024.	1.9	16
303	Coordination and Haptotropic Migration of Cr(CO)₃in Polycyclic Aromatic Hydrocarbons:â€‰ The Effect of the Size and the Curvature of the Substrate. Journal of Physical Chemistry A, 2008, 112, 1202-1213.	1.1	33
304	Intramolecular Haptotropic Rearrangements of the Tricarbonylchromium Complex in Small Polycyclic Aromatic Hydrocarbons. Organometallics, 2008, 27, 5230-5240.	1.1	31
305	Chemical Reactivity of D3h C78 (Metallo)Fullerene: Regioselectivity Changes Induced by Sc3N Encapsulation. Journal of the American Chemical Society, 2008, 130, 6206-6214.	6.6	75
306	Chapter 3 The breakdown of the maximum hardness and minimum polarizability principles for nontotally symmetric vibrations. Theoretical and Computational Chemistry, 2007, , 31-45.	0.2	2

#	Article	IF	Citations
307	Chapter 10 Electronic structure and reactivity of aromatic metal clusters. Theoretical and Computational Chemistry, 2007, 19, 203-218.	0.2	0
308	Mechanistic Insights into the Chemistry of Ru(II) Complexes Containing Cl and DMSO Ligands. Inorganic Chemistry, 2007, 46, 10707-10716.	1.9	53
309	New Solids Based on B₁₂N₁₂ Fullerenes. Journal of Physical Chemistry C, 2007, 111, 13354-13360.	1.5	72
310	Electron sharing indexes at the correlated level. Application to aromaticity calculations. Faraday Discussions, 2007, 135, 325-345.	1.6	203
311	Highly polar bonds and the meaning of covalency and ionicityâ€"structure and bonding of alkali metal hydride oligomers. Faraday Discussions, 2007, 135, 451-468.	1.6	19
312	Theoretical Study of the Reaction Mechanisms Involved in the Thermal Intramolecular Reactions of 1,6-Fullerenynes. Journal of Physical Chemistry A, 2007, 111, 5253-5258.	1.1	12
313	Aromaticity of Distorted Benzene Rings:â€‰ Exploring the Validity of Different Indicators of Aromaticity. Journal of Physical Chemistry A, 2007, 111, 4513-4521.	1.1	102
314	Didehydrophenanthrenes:â€‰ Structure, Singletâ^'Triplet Splitting, and Aromaticity. Journal of Physical Chemistry A, 2007, 111, 5063-5070.	1.1	39
315	Table Salt and Other Alkali Metal Chloride Oligomers:â€‰ Structure, Stability, and Bonding. Inorganic Chemistry, 2007, 46, 5411-5418.	1.9	17
316	Fast O2Binding at Dicopper Complexes Containing Schiff-Base Dinucleating Ligands. Inorganic Chemistry, 2007, 46, 4997-5012.	1.9	43
317	Properties of Aromaticity Indices Based on the One-Electron Density Matrix. Journal of Physical Chemistry A, 2007, 111, 6521-6525.	1.1	118
318	Polycyclic Benzenoids:Â Why Kinked is More Stable than Straight. Journal of Organic Chemistry, 2007, 72, 1134-1142.	1.7	197
319	On the quality of the hardness kernel and the Fukui function to evaluate the global hardness. Journal of Computational Chemistry, 2007, 28, 574-583.	1.5	48
320	Covalentversus ionic bonding in alkalimetal fluoride oligomers. Journal of Computational Chemistry, 2007, 28, 238-250.	1.5	18
321	Energy landscapes of nucleophilic substitution reactions: A comparison of density functional theory and coupled cluster methods. Journal of Computational Chemistry, 2007, 28, 1551-1560.	1.5	89
322	Electron delocalization and aromaticity measures within the HÃ¼ckel molecular orbital method. Computational and Theoretical Chemistry, 2007, 811, 3-11.	1.5	46
323	Aromaticity changes along the reaction coordinate connecting the cyclobutadiene dimer to cubane and the benzene dimer to hexaprismane. Structural Chemistry, 2007, 18, 773-783.	1.0	18
324	The proton transfer reaction in malonaldehyde derivatives: Substituent effects and quasi-aromaticity of the proton bridge. Chemical Physics, 2007, 342, 43-54.	0.9	43

#	Article	IF	Citations
325	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.	1.7	57
326	Copper(II) Hexaaza Macrocyclic Binuclear Complexes Obtained from the Reaction of Their Copper(I) Derivates and Molecular Dioxygen. Inorganic Chemistry, 2006, 45, 3569-3581.	1.9	61
327	Pseudo-Jahnâ^'Teller Effect as the Origin of the Exalted Frequency of the b2u KekulÃ© Mode in the 1B2u Excited State of Benzene. Journal of Physical Chemistry A, 2006, 110, 11219-11222.	1.1	23
328	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.	1.6	70
329	Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. Journal of Physical Chemistry A, 2006, 110, 12249-12258.	1.1	52
330	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.	1.1	76
331	Interplay between Intramolecular Resonance-Assisted Hydrogen Bonding and Aromaticity in o-Hydroxyaryl Aldehydes. Journal of Organic Chemistry, 2006, 71, 5241-5248.	1.7	110
332	A Novel Exploration of the Hartreeâ€“Fock Homolytic Bond Dissociation Problem in the Hydrogen Molecule by Means of Electron Localization Measures. Journal of Chemical Education, 2006, 83, 1243.	1.1	19
333	Gas-Phase Structures, Rotational Barriers, and Conformational Properties of Hydroxyl and Mercapto Derivatives of Cyclohexa-2,5-dienone and Cyclohexa-2,5-dienthione. Journal of Physical Chemistry A, 2006, 110, 8901-8911.	1.1	8
334	New Ru Complexes Containing the N-Tridentate bpea and Phosphine Ligands:Â Consequences of Meridional vs Facial Geometry. Inorganic Chemistry, 2006, 45, 10520-10529.	1.9	41
335	Covalency in Highly Polar Bonds. Structure and Bonding of Methylalkalimetal Oligomers (CH3M)n (M) Tj ETQq1 1 0.784314 rgBT /Ov	2.3	48
336	Redox-Controlled Molecular Flipper Based on a Chiral Cu Complex. Inorganic Chemistry, 2006, 45, 9643-9645.	1.9	10
337	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.	1.2	39
338	Electron localization function at the correlated level. Journal of Chemical Physics, 2006, 125, 024301.	1.2	135
339	Intramolecular Ene Reaction of 1,6-Fullerenynes:â€‰ A New Synthesis of Allenes. Organic Letters, 2006, 8, 5959-5962.	2.4	33
340	O2Chemistry of Dicopper Complexes with Alkyltriamine Ligands. Comparing Synergistic Effects on O2Binding. Inorganic Chemistry, 2006, 45, 5239-5241.	1.9	26
341	Molecular Structure and Bonding of Copper Cluster Monocarbonyls CunCO (n= 1â^'9). Journal of Physical Chemistry B, 2006, 110, 6526-6536.	1.2	97
342	Are nucleus-independent (NICS) and 1H NMR chemical shifts good indicators of aromaticity in Ï€-stacked polyfluorenes?. Chemical Physics Letters, 2006, 428, 191-195.	1.2	33

#	Article	IF	Citations
343	Nucleus-independent chemical shift (NICS) profiles in a series of monocyclic planar inorganic compounds. Journal of Organometallic Chemistry, 2006, 691, 4359-4366.	0.8	155
344	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.	1.1	28
345	Structure and bonding of methyl alkali metal molecules. Journal of Molecular Modeling, 2006, 12, 563-568.	0.8	11
346	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.	0.1	0
347	Atropisomeric Discrimination in New RuII Complexes Containing theC2-Symmetric Didentate Chiral Phenyl-1,2-bisoxazolinic Ligand. Chemistry - A European Journal, 2006, 12, 2798-2807.	1.7	30
348	Hydrogenâ€“Hydrogen Bonding in Planar Biphenyl, Predicted by Atoms-In-Molecules Theory, Does Not Exist. Chemistry - A European Journal, 2006, 12, 2889-2895.	1.7	314
349	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.	1.7	216
350	Thermal [2+2] Intramolecular Cycloadditions of Fuller-1,6-enynes. Angewandte Chemie - International Edition, 2006, 45, 1439-1442.	7.2	53
351	Regiospecific Cï£¿H Bond Activation: Reversible H/D Exchange Promoted by CuI Complexes with Triazamacrocyclic Ligands. Angewandte Chemie - International Edition, 2006, 45, 2941-2944.	7.2	42
352	Electron Fluctuation in Pericyclic and Pseudopericyclic Reactions. ChemPhysChem, 2006, 7, 111-113.	1.0	45
353	Chemical bonding in transition metal carbene complexes. Journal of Organometallic Chemistry, 2005, 690, 6178-6204.	0.8	206
354	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
355	Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1â^'9). Journal of Organic Chemistry, 2005, 70, 2509-2521.	1.7	195
356	Oxidative addition of the ethane Cï£¿C bond to Pd. Anab initiobenchmark and DFT validation study. Journal of Computational Chemistry, 2005, 26, 1006-1020.	1.5	69
357	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.	1.5	133
358	Aromaticity Analysis of Lithium Cation/ Ï€ Complexes of Aromatic Systems. ChemPhysChem, 2005, 6, 2552-2561.	1.0	46
359	Regioselective Intramolecular Pauson-Khand Reactions of C60: An Electrochemical Study and Theoretical Underpinning. Chemistry - A European Journal, 2005, 11, 2716-2729.	1.7	58
360	Fine-Tuning the Electronic Properties of Highly Stable Organometallic CuIII Complexes Containing Monoanionic Macrocyclic Ligands. Chemistry - A European Journal, 2005, 11, 5146-5156.	1.7	106

#	Article	IF	Citations
361	The Breakdown of the Minimum Polarizability Principle in Vibrational Motions as an Indicator of the Most Aromatic Center. Chemistry - A European Journal, 2005, 11, 6024-6031.	1.7	15
362	Basis set effects on the energy and hardness profiles of the hydrogen fluoride dimer. Journal of Chemical Sciences, 2005, 117, 549-554.	0.7	4
363	Ab initio and DFT modeling of stereoselective deamination of aziridines by nitrosyl chloride. International Journal of Quantum Chemistry, 2005, 102, 139-146.	1.0	9
364	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.	0.9	147
365	Calculation of Franckâ€“Condon factors including anharmonicity: Simulation of the C2H4+XÌƒB3u2â†C2H4XÌƒAg1 band in the photoelectron spectrum of ethylene. Journal of Chemical Physics, 2005, 122, 184104.	1.2	25
366	The aromatic fluctuation index (FLU): A new aromaticity index based on electron delocalization. Journal of Chemical Physics, 2005, 122, 014109.	1.2	396
367	An assessment of a simple hardness kernel approximation for the calculation of the global hardness in a series of Lewis acids and bases. Computational and Theoretical Chemistry, 2005, 727, 139-148.	1.5	31
368	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.	23.0	661
369	Local Aromaticity of the Lowest-Lying Singlet States of [n]Acenes (n = 6â€“9). Journal of Physical Chemistry A, 2005, 109, 10629-10632.	1.1	68
370	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.	0.8	32
371	Generalizing the Breakdown of the Maximum Hardness and Minimum Polarizabilities Principles for Nontotally Symmetric Vibrations to Non-Ï€-Conjugated Organic Molecules. Journal of Physical Chemistry A, 2005, 109, 615-621.	1.1	26
372	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.	1.2	17
373	Comparison of the AIM Delocalization Index and the Mayer and Fuzzy Atom Bond Orders. Journal of Physical Chemistry A, 2005, 109, 9904-9910.	1.1	169
374	Diastereoselective Synthesis of Fulleropyrrolidines from Suitably Functionalized Chiral Cyclobutanes. Journal of Organic Chemistry, 2005, 70, 6929-6932.	1.7	22
375	Theoretical Study of the Highly Diastereoselective 1,3-Dipolar Cycloaddition of 1,4-Dihydropyridine-Containing Azomethine Ylides to [60]Fullerene (Prato's Reaction). Journal of Organic Chemistry, 2005, 70, 3256-3262.	1.7	36
376	The hardness profile as a tool to detect spurious stationary points in the potential energy surface. Journal of Chemical Physics, 2004, 120, 10914-10924.	1.2	32
377	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.	1.2	60
378	Relation between the Substituent Effect and Aromaticity. Journal of Organic Chemistry, 2004, 69, 6634-6640.	1.7	177

#	Article	IF	Citations
379	Analysis of electronic delocalization in buckminsterfullerene (C60). International Journal of Quantum Chemistry, 2004, 98, 361-366.	1.0	23
380	Second-order atomic Fukui indices from the electron-pair density in the framework of the atoms in molecules theory. Journal of Computational Chemistry, 2004, 25, 439-446.	1.5	13
381	Discrepancy Between Common Local Aromaticity Measures in a Series of Carbazole Derivatives. ChemInform, 2004, 35, no.	0.1	0
382	Ground and Low-Lying States of Cu2+â€"H2O. A Difficult Case for Density Functional Methods.. ChemInform, 2004, 35, no.	0.1	0
383	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.	1.2	73
384	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.	1.7	113
385	Quantum Chemical Study of the Reactivity of C60HR and C60(CHR) Derivatives. Journal of Organic Chemistry, 2004, 69, 2374-2380.	1.7	9
386	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.	1.1	85
387	Discrepancy between common local aromaticity measures in a series of carbazole derivatives. Physical Chemistry Chemical Physics, 2004, 6, 314-318.	1.3	106
388	Stereodiscrimination in Phosphanylthiolato Nickel(II) Complexes. European Journal of Inorganic Chemistry, 2003, 2003, 4147-4151.	1.0	14
389	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes.. ChemInform, 2003, 34, no.	0.1	0
390	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.	1.7	396
391	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes. Chemistry - A European Journal, 2003, 9, 1113-1122.	1.7	125
392	Electron pairing analysis of the Fischer-type chromiumâ€"carbene complexes (CO)5Crˆ...C(X)R (X=H, OH,) Tj ETQq0 0 0 rgBT /Overlock	0.9	18
393	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.	1.2	74
394	Evaluation of the Analogy between Exceptions to the Generalized Maximum Hardness Principle for Non-Totally-Symmetric Vibrations and the Pseudo-Jahnâ˜Teller Effect. Journal of Physical Chemistry A, 2003, 107, 7337-7339.	1.1	18
395	Dinuclear Copper(I) Complexes with Hexaaza Macrocyclic Dinucleating Ligands:â€‰ Structure and Dynamic Properties. Inorganic Chemistry, 2003, 42, 4456-4468.	1.9	21
396	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.	1.2	105

#	Article	IF	Citations
397	Relations among several nuclear and electronic density functional reactivity indexes. Journal of Chemical Physics, 2003, 119, 9393-9400.	1.2	22
398	Are the maximum hardness and minimum polarizability principles always obeyed in nontotally symmetric vibrations?. Journal of Chemical Physics, 2002, 117, 10561-10570.	1.2	77
399	BIELECTRONIC DENSITIES: ANALYSIS AND APPLICATIONS IN MOLECULAR STRUCTURE AND CHEMICAL REACTIVITY. , 2002, , 831-870.		2
400	Isolation and Characterization of Four Isomers of a C60Bisadduct with a TTF Derivative. Study of Their Radical Ions. Journal of Organic Chemistry, 2002, 67, 566-575.	1.7	22
401	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.	1.1	80
402	Global Hardness Evaluation Using Simplified Models for the Hardness Kernel. Journal of Physical Chemistry A, 2002, 106, 4632-4638.	1.1	29
403	Initial convergence of the perturbation series expansion for vibrational nonlinear optical properties. Journal of Chemical Physics, 2002, 116, 5363-5373.	1.2	43
404	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.	1.3	51
405	Electron localization and delocalization in open-shell molecules. Journal of Computational Chemistry, 2002, 23, 1347-1356.	1.5	34
406	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.	0.5	187
407	Electron-pairing analysis from localization and delocalization indices in the framework of the atoms-in-molecules theory. Theoretical Chemistry Accounts, 2002, 108, 214-224.	0.5	175
408	PRISTINE AND SILICON-SUBSTITUTED SMALL-CARBON-CLUSTERS AND FULLERENES: ELECTRONIC STRUCTURE AND REACTIVITY. , 2002, , 1367-1420.		2
409	A Theoretical Study of Steric and Electronic Effects in the Rhodium-Catalyzed Carbonylation Reactions. Journal of the American Chemical Society, 2001, 123, 12294-12302.	6.6	63
410	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.	6.6	112
411	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.	1.7	91
412	Theoretical Study of the Proton Transfer between Water and [FeH(CO)4]- in Aqueous Solution and Relevance to the Water-Gas Shift Reaction Catalyzed by Iron Pentacarbonyl in the Condensed Phase. Organometallics, 2001, 20, 1310-1316.	1.1	15
413	New Insights in Chemical Reactivity by Means of Electron Pairing Analysis. Journal of Physical Chemistry A, 2001, 105, 2052-2063.	1.1	34
414	Effects of Solvation on the Pairing of Electrons in a Series of Simple Molecules and in the Menshutkin Reaction. Journal of Physical Chemistry A, 2001, 105, 6249-6257.	1.1	32

#	Article	IF	Citations
415	Density functional theory study of the structures and stabilities of CuO and CuO3. International Journal of Quantum Chemistry, 2001, 81, 162-168.	1.0	11
416	Parametrization of the Becke3-LYP hybrid functional for a series of small molecules using quantum molecular similarity techniques. Journal of Computational Chemistry, 2001, 22, 1666-1678.	1.5	21
417	Theoretical characterization of intramolecular proton transfer in the ground and the lowest-lying triplet excited states of 1-amino-3-propenal: a methodological comparison. Journal of Computational Chemistry, 2000, 21, 257-269.	1.5	11
418	Substituent effects on the intramolecular proton transfer in the ground and lowest-lying singlet excited states of salicylaldimine. Chemical Physics, 2000, 260, 53-64.	0.9	22
419	The [2+1] Cycloaddition of Singlet Oxycarbonylnitrenes to C 60. Journal of Molecular Modeling, 2000, 6, 205-212.	0.8	14
420	Theoretical Studies of Some Transition-Metal-Mediated Reactions of Industrial and Synthetic Importance. Chemical Reviews, 2000, 100, 439-494.	23.0	371
421	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.	1.1	79
422	Weighing Different Mechanistic Proposals for the DÃ¶tz Reaction:Â A Density Functional Study. Journal of the American Chemical Society, 1999, 121, 1309-1316.	6.6	37
423	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.	1.1	78
424	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.	1.1	55
425	The Hammond Postulate and the Principle of Maximum Hardness in Some Intramolecular Rearrangement Reactions. Journal of Physical Chemistry A, 1999, 103, 8847-8852.	1.1	62
426	Optimizing hybrid density functionals by means of quantum molecular similarity techniques. Advances in Molecular Similarity, 1999, , 187-203.	0.5	2
427	Exploring the possibility of a bimolecular reaction channel for the F2SS/FSSF rearrangement process. Computational and Theoretical Chemistry, 1998, 455, 123-129.	1.5	5
428	The use of ab initio quantum molecular self-similarity measures to analyze electronic charge density distributions. International Journal of Quantum Chemistry, 1998, 58, 361-372.	1.0	31
429	Intramolecular proton transfer in the ground and the two lowest-lying singlet excited states of 1-amino-3-propenal and related species. Chemical Physics, 1998, 234, 1-19.	0.9	24
430	Low-lying electronic states and molecular structure of Fe2O2. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2877-2881.	1.7	9
431	Density Functional Study on the Preactivation Scenario of the DÃ¶tz Reaction:â€‰ Carbon Monoxide Dissociation versus Alkyne Addition as the First Reaction Step. Organometallics, 1998, 17, 1492-1501.	1.1	34
432	Dielsâ€™Alder Cycloadditions of 1,3-Butadiene to Polycyclic Aromatic Hydrocarbons (PAH). Quantifying the Reactivity Likeness of Bowl-Shaped PAHs to C60. Journal of Organic Chemistry, 1998, 63, 7556-7558.	1.7	24

#	Article	IF	Citations
433	Theoretical Study on the Thermodynamics of the Elimination of Formic Acid in the Last Step of the Hydrogenation of CO2Catalyzed by Rhodium Complexes in the Gas Phase and Supercritical CO2. Organometallics, 1998, 17, 3164-3168.	1.1	39
434	Density Functional Study of the [2+2]- and [2+3]-Cycloaddition Mechanisms for the Osmium-Catalyzed Dihydroxylation of Olefins. Organometallics, 1997, 16, 13-19.	1.1	122
435	Coordinative Behavior of the CNCN Ligand. Experimental and Density Functional Study of Spectroscopic Properties and Bonding in the Cr(CO)5CNCN Complex. Organometallics, 1997, 16, 2254-2262.	1.1	10
436	Preparation and characterization of pyridinium-n-carboxylate trioxochromate (VI) (n=3, 4) and pyridinium-4-carboxylic pyridine-4 carboxylate trioxochromate (VI) hemihydrate. Inorganica Chimica Acta, 1997, 258, 53-63.	1.2	10
437	Low-lying electronic states and molecular structure of FeO2 and FeO2â¯. Chemical Physics Letters, 1997, 274, 411-421.	1.2	26
438	Theoretical Study on Acetaldehyde and Ethanol Elimination from the Hydrogenation of CH3(O)CCo(CO)3. Organometallics, 1996, 15, 2611-2618.	1.1	49
439	Theoretical Study of the Regioselectivity of Successive 1,3-Butadiene Dielsâ¯Alder Cycloadditions to C60. Journal of the American Chemical Society, 1996, 118, 8920-8924.	6.6	37
440	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.	1.2	54
441	An assessment of density functional theory on evaluating activation barriers for small organic gas-phase rearrangement reactions. Computational and Theoretical Chemistry, 1996, 362, 163-173.	1.5	27
442	Analysis of the changes on the potential energy surface of Menshutkin reactions induced by external perturbations. Computational and Theoretical Chemistry, 1996, 371, 171-183.	1.5	26
443	Effect of Solvation on the Charge Distribution of a Series of Anionic, Neutral, and Cationic Species. A Quantum Molecular Similarity Study. The Journal of Physical Chemistry, 1996, 100, 606-610.	2.9	27
444	Exploring chromium (VI) dioxodihalides chemistry: Is density functional theory the most suitable tool?. Journal of Chemical Physics, 1996, 104, 9499-9510.	1.2	28
445	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
446	The use of ab initio quantum molecular selfâ€similarity measures to analyze electronic charge density distributions. International Journal of Quantum Chemistry, 1996, 58, 361-372.	1.0	25
447	How similar are HF, MP2, and DFT charge distributions in the Cr(CO)6 complex?. Advances in Molecular Similarity, 1996, , 167-186.	0.5	2
448	Theoretical investigation of the relative stabilities ofXSSXandX2SS isomers (X= F, Cl, H, and CH3). Journal of Computational Chemistry, 1995, 16, 465-477.	1.5	52
449	Molecular Size and Pyramidalization: Two Keys for Understanding the Reactivity of Fullerenes. The Journal of Physical Chemistry, 1995, 99, 10752-10758.	2.9	50
450	Ab initio study of the HCO 3 ? /H2O exchange in the (NH3)3 ZnII(HCO 3 ?) complex. Theoretica Chimica Acta, 1995, 91, 333-351.	0.9	1

#	Article	IF	Citations
451	AM1 study of a substituent transfer by means of a Dielsâ€“Alder and retro-Dielsâ€“Alder tandem reaction. Journal of the Chemical Society Perkin Transactions II, 1995, , 605-608.	0.9	5
452	Foundations and recent developments on molecular quantum similarity. Topics in Current Chemistry, 1995, , 31-62.	4.0	72
453	An AM1 study of the reactivity of buckminsterfullerene (C60) in a Diels-Alder model reaction. Chemical Physics Letters, 1994, 231, 325-330.	1.2	49
454	On the calculation ofab initioquantum molecular similarities for large systems: Fitting the electron density. Journal of Computational Chemistry, 1994, 15, 1113-1120.	1.5	46
455	A quantum chemical AM1 study of a Dielsâ€“Alder and retro-Dielsâ€“Alder tandem reaction. Journal of the Chemical Society Perkin Transactions II, 1994, , 281-284.	0.9	8
456	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.	6.6	54
457	Ab Initio Quantum Molecular Similarity Measures on Metal-Substituted Carbonic Anhydrase (MIICA, M) Tj ETQq1 1 0.784314 rgBT /Over 1047-1053.	2.8	25
458	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.	6.6	70
459	Valence-bond calculations on ZNO and HGO using integrals computed through the semiempiricalAM1 method. International Journal of Quantum Chemistry, 1992, 44, 887-895.	1.0	2
460	Ab initio study of the effect of external perturbations in the dissociation of CH3Cl. Computational and Theoretical Chemistry, 1992, 255, 283-296.	1.5	8
461	Theoretical Study of the Catalyzed Hydration of CO2 by Carbonic Anhydrase: A Brief Overview.. , 1992, , 263-298.		2
462	Anion binding and pentacoordination in zinc(II) complexes. Inorganic Chemistry, 1991, 30, 2523-2527.	1.9	31
463	Analysis of solvent effects on the Menshutkin reaction. Journal of the American Chemical Society, 1991, 113, 2873-2879.	6.6	123
464	Analysis in terms of valence-bond structures of environmental effects on the electronic structure of molecules. International Journal of Quantum Chemistry, 1991, 40, 511-525.	1.0	7
465	Ab initiostudy of substituent effect on the addition of hydrogen fluoride to fluoroethylenes. Journal of Computational Chemistry, 1990, 11, 170-180.	1.5	13
466	Aromaticity Analysis by Means of the Quantum Theory of Atoms in Molecules. , 0, , 399-423.		6
467	One Century of Physical Organic Chemistry: The Menshutkin Reaction. Progress in Physical Organic Chemistry, 0, , 1-182.	1.2	47
468	A Rh(I)â€Catalyzed Cascade Cyclization of 1,5â€Bisallenes and Alkynes for the Formation of cisâ€3,4â€Arylvinyl Pyrrolidines and Cyclopentanes. Advanced Synthesis and Catalysis, 0, , .	2.1	3

#	Article	IF	Citations
469	Aromaticity and Extrusion of Benzenoids Linked to [o â€COSAN] ^{âˆ’} : Clar Has the Answer. Angewandte Chemie, 0, , .	1.6	3