

Miquel SolÀ

List of Publications by Year in descending order

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papers

20,593
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11908

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docs citations

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times ranked

12536
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#	ARTICLE	IF	CITATIONS
1	Initiating Electron Transfer in Doubly Curved Nanographene Upon Supramolecular Complexation of C ₆₀ . <i>Angewandte Chemie</i> , 2022, 134, .	1.6	9
2	Initiating Electron Transfer in Doubly Curved Nanographene Upon Supramolecular Complexation of C ₆₀ . <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	48
3	Effect of Diamine Bridge on Reactivity of Tetradentate ONNO Nickel(II) Complexes. <i>ChemPhysChem</i> , 2022, 23, .	1.0	0
4	Enhancing the Catalytic Performance of Group I, II Metal Halides in the Cycloaddition of CO ₂ to Epoxides under Atmospheric Conditions by Cooperation with Homogeneous and Heterogeneous Highly Nucleophilic Aminopyridines: Experimental and Theoretical Study. <i>Journal of Organic Chemistry</i> , 2022, 87, 2873-2886.	1.7	25
5	Path-dependency of energy decomposition analysis & the elusive nature of bonding. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 2344-2348.	1.3	27
6	Nitrogen-doped molecular bowls as electron donors in photoinduced electron transfer reactions. <i>Nanoscale Advances</i> , 2022, 4, 2180-2188.	2.2	6
7	Aromaticity and Extrusion of Benzenoids Linked to [10]CPP@COSAN: Clar Has the Answer. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	12
8	Successive Diels-Alder Cycloadditions of Cyclopentadiene to [10]CPP@C ₆₀ : A Computational Study. <i>Journal of Organic Chemistry</i> , 2022, 87, 5149-5157.	1.7	6
9	Highly Selective Synthesis of Seven-Membered Azaspiro Compounds by a Rh(I)-Catalyzed Cycloisomerization/Diels-Alder Cascade of 1,5-Bisallenenes. <i>Journal of Organic Chemistry</i> , 2022, 87, 5279-5286.	1.7	7
10	The importance of the bite angle of metal(III) salen catalysts in the sequestration of CO ₂ with epoxides in mild conditions. <i>Green Chemical Engineering</i> , 2022, 3, 180-187.	3.3	18
11	Knölker Iron Catalysts for Hydrogenation Revisited: A Nonspectator Solvent and Fine-Tuning. <i>Organometallics</i> , 2022, 41, 1204-1215.	1.1	14
12	Three-Dimensional Fully π -Conjugated Macrocycles: When 3D-Aromatic and When 2D-Aromatic-in-3D?. <i>Journal of the American Chemical Society</i> , 2022, 144, 8560-8575.	6.6	28
13	Cage size effects on the encapsulation of P ₂ by fullerenes. <i>Journal of Computational Chemistry</i> , 2022, .	1.5	1
14	The Hunter Falls Prey: Photoinduced Oxidation of C ₆₀ in Inclusion Complex with Perfluorocycloparaphenylene. <i>ChemPhysChem</i> , 2022, 23, .	1.0	9
15	Aromaticity of Singlet and Triplet Boron Disk-like Clusters: A Test for Electron Counting Aromaticity Rules. <i>Inorganic Chemistry</i> , 2022, 61, 10116-10125.	1.9	3
16	Aromaticity rules. <i>Nature Chemistry</i> , 2022, 14, 585-590.	6.6	55
17	3D and 2D aromatic units behave like oil and water in the case of benzocarborane derivatives. <i>Nature Communications</i> , 2022, 13, .	5.8	23
18	Mechanistic Studies of Transition-Metal-Catalyzed [2 + 2 + 2] Cycloaddition Reactions. <i>Chemical Reviews</i> , 2021, 121, 1894-1979.	23.0	125

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19	Aromaticity of nucleic acid bases. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1509.	6.2	7
20	Cycloaddition of CO ₂ 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 π -Aromatic Circuits. Chemistry - A European Journal, 2021, 27, 802-808.	1.7	9
22	An unprecedented π -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 $H_{1/4}^{\text{ckel}}$ -Baird Hybrid Aromatic Character of Pro π -Aromatic Quinoidal Compounds**. Angewandte Chemie, 2021, 133, 10343-10353.	1.6	3
30	Guidelines for Tuning the Excited State $H_{1/4}^{\text{ckel}}$ -Baird Hybrid Aromatic Character of Pro π -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 (C ₆₀ and C ₇₀) 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 ⁺ @C ₆₀ @C ₂₄₀ 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]CPP-Based Inclusion Complexes of Charged Fullero-pyrrolidines. Effect of the Charge Location on the Photoinduced Electron Transfer. <i>Chemistry - A European Journal</i> , 2021, 27, 8737-8744.	1.7	10
38	Synthesis of Fused Dihydroazepine Derivatives of Fullerenes by a Rh-Catalyzed Cascade Process. <i>Advanced Synthesis and Catalysis</i> , 2021, 363, 3835-3844.	2.1	8
39	Chelation enforcing a dual gold configuration in the catalytic hydroxyphenoxylation of alkynes. <i>Applied Organometallic Chemistry</i> , 2021, 35, e6362.	1.7	5
40	Unexpected Disparity in Photoinduced Reactions of C ₆₀ and C ₇₀ in Water with the Generation of O ₂ ^{•-} or ¹ O ₂ . <i>Jacs Au</i> , 2021, 1, 1601-1611.	3.6	9
41	Predictive Catalysis in Olefin Metathesis with Ru-Based Catalysts with Annulated C ₆₀ Fullerenes in the N-heterocyclic Carbenes. <i>Chemistry - A European Journal</i> , 2021, 27, 18074-18083.	1.7	3
42	Evaluation of charge-transfer rates in fullerene-based donor-acceptor dyads with different density functional approximations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5376-5384.	1.3	18
43	The Relative Stability of Indole Isomers Is a Consequence of the Glidewell-Lloyd Rule. <i>Journal of Physical Chemistry A</i> , 2021, 125, 230-234.	1.1	16
44	Photoinduced electron transfer in non-covalent complexes of C ₆₀ and phosphangulene oxide derivatives. <i>Dalton Transactions</i> , 2021, 50, 16214-16222.	1.6	3
45	Cage-Cage Interaction: Boron Cluster-Based Noncovalent Bond and Its Applications in Solid-State Materials. <i>Jacs Au</i> , 2021, 1, 2047-2057.	3.6	5
46	Fast and Simple Evaluation of the Catalysis and Selectivity Induced by External Electric Fields. <i>ACS Catalysis</i> , 2021, 11, 14467-14479.	5.5	14
47	Reactivity of the superhalogen/superalkali ion encapsulating C ₆₀ fullerenes. <i>Dalton Transactions</i> , 2021, 51, 203-210.	1.6	2
48	Cyclo[18]carbon: the smallest all-carbon electron acceptor. <i>Chemical Communications</i> , 2020, 56, 352-355.	2.2	78
49	Do Carbon Nanocages Behave as Nanoscopic Faraday Cages? A Comparison of the Reactivity of C ₆₀ , C ₂₄₀ , C ₆₀ @C ₂₄₀ , Li ⁺ @C ₆₀ , Li ⁺ @C ₂₄₀ , and Li ⁺ @C ₆₀ @C ₂₄₀ . <i>Chemistry - A European Journal</i> , 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. <i>Catalysis Today</i> , 2020, 358, 278-283.	2.2	9
51	Iodane-Guided ortho-H Allylation. <i>Angewandte Chemie</i> , 2020, 132, 20376-20382.	1.6	2
52	Bingel-Hirsch Addition of Diethyl Bromomalonate to Ion-Encapsulated Fullerenes M@C ₆₀ (M=Li, Na, K). <i>Journal of Physical Chemistry C</i> , 2020, 124, 11000-11006.	1.7	6
53	Iodane-Guided ortho-H Allylation. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 20201-20207.	7.2	8
54	Probing the Origin of Adaptive Aromaticity in 16-Valence-Electron Metallapentalenes. <i>Chemistry - A European Journal</i> , 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 nanotube@C ₇₀ inclusion complexes: phenine <i>vs</i> nanographene nanotubes. Chemical Communications, 2020, 56, 12624-12627.	2.2	16
58	Electron Transfer in a Li ⁺ -Doped Zn-Porphyrin@[10]CPP@Fullerene 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 B ₁₂ doped with beryllium and/or carbon. Physical Chemistry Chemical Physics, 2020, 22, 12245-12259.	1.3	12
61	Triquinoline- <i>vs</i> Fullerene-Based Cycloparaphenylene Ionic Complexes: Comparison of Photoinduced Charge-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 16-Valence-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 @Cage...@ Bond: A Non-covalent Interaction between Boron Clusters and Aromatic Rings and Its Applications. Angewandte Chemie, 2020, 132, 9103-9110.	1.6	7
67	The <i>nido</i> @Cage...@ Bond: A Non-covalent Interaction between Boron Clusters and Aromatic Rings and Its Applications. Angewandte Chemie - International Edition, 2020, 59, 9018-9025.	7.2	32
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 Dienes 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/Diels-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. <i>Organometallics</i> , 2019, 38, 2853-2862.	1.1	34
74	Nine questions on energy decomposition analysis. <i>Journal of Computational Chemistry</i> , 2019, 40, 2248-2283.	1.5	113
75	Special Collection: Computational Chemistry. <i>ChemistryOpen</i> , 2019, 8, 814-816.	0.9	3
76	Mechanism of the Manganese-Pincer-Catalyzed Acceptorless Dehydrogenative Coupling of Nitriles and Alcohols. <i>Journal of the American Chemical Society</i> , 2019, 141, 2398-2403.	6.6	69
77	Hypsochromic solvent shift of the charge separation band in ionic donor-acceptor Li ⁺ @C ₆₀ . [10]CPP. <i>Chemical Communications</i> , 2019, 55, 11195-11198.	2.2	23
78	Exploiting the Aromatic Chameleon Character of Fulvenes for Computational Design of Baird-Aromatic Triplet Ground State Compounds. <i>Chemistry - an Asian Journal</i> , 2019, 14, 1870-1878.	1.7	13
79	Regioselectivity in Diels-Alder Cycloadditions of C ₆₀ Fullerene with a Triplet Ground State. <i>Journal of Organic Chemistry</i> , 2019, 84, 9017-9024.	1.7	7
80	Photoinduced Charge Shift in Li ⁺ -Doped Giant Nested Fullerenes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16525-16532.	1.5	13
81	Effect of Exocyclic Substituents and π -System Length on the Electronic Structure of Chichibabin Diradical(oid)s. <i>ACS Omega</i> , 2019, 4, 10845-10853.	1.6	10
82	Innen-Äußertitelbild: All-Fullerene Electron Donor-Acceptor Conjugates (<i>Angew. Chem.</i> 21/2019). <i>Angewandte Chemie</i> , 2019, 131, 7217-7217.	1.6	1
83	All-Fullerene Electron Donor-Acceptor Conjugates. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 6932-6937.	7.2	35
84	Is Excited-State Aromaticity a Driving Force for Planarization of Dibenzannelated π -Electron Heterocycles?. <i>ChemPlusChem</i> , 2019, 84, 712-721.	1.3	38
85	All-Fullerene Electron Donor-Acceptor Conjugates. <i>Angewandte Chemie</i> , 2019, 131, 7006-7011.	1.6	13
86	Electron Delocalization in Planar Metallacycles: Hückel or Möbius Aromatic?. <i>ChemistryOpen</i> , 2019, 8, 219-227.	0.9	49
87	The Coulomb Hole of the Ne Atom. <i>ChemistryOpen</i> , 2019, 8, 411-417.	0.9	6
88	Open-shell jellium aromaticity in metal clusters. <i>Chemical Communications</i> , 2019, 55, 5559-5562.	2.2	15
89	Decomposition of the electronic activity in competing [5,6] and [6,6] cycloaddition reactions between C ₆₀ and cyclopentadiene. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5039-5048.	1.3	11
90	Photoinduced electron transfer and unusual environmental effects in fullerene-Zn-porphyrin-BODIPY triads. <i>Physical Chemistry Chemical Physics</i> , 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 <i>o</i> -Hydroxyaldehyde Groups: The Importance of Topology. <i>Journal of Organic Chemistry</i> , 2019, 84, 15538-15548.	1.7	13
92	Connecting and combining rules of aromaticity. Towards a unified theory of aromaticity. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1404.	6.2	37
93	Peculiar Photoinduced Electron Transfer in Porphyrin–Fullerene Akamptisomers. <i>Chemistry - A European Journal</i> , 2019, 25, 2577-2585.	1.7	9
94	(Invited) Photoinduced Charge Separation in Several Dyads Involving Fullerenes. <i>ECS Meeting Abstracts</i> , 2019, , .	0.0	0
95	52 GAMES WITH THE PERIODIC TABLE AND BEYOND. , 2019, , .		0
96	Rationalizing the Regioselectivity of the Diels–Alder Biscycloaddition of Fullerenes. <i>Journal of Organic Chemistry</i> , 2018, 83, 3285-3292.	1.7	11
97	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. <i>Chemistry - A European Journal</i> , 2018, 24, 9853-9859.	1.7	28
98	Reliable charge assessment on encapsulated fragment for endohedral systems. <i>Scientific Reports</i> , 2018, 8, 2882.	1.6	5
99	Tuning the Strength of the Resonance-Assisted Hydrogen Bond in <i>o</i> -Hydroxybenzaldehyde by Substitution in the Aromatic Ring ¹ . <i>Journal of Physical Chemistry A</i> , 2018, 122, 2279-2287.	1.1	28
100	On the regioselectivity of the Diels–Alder cycloaddition to C ₆₀ in high spin states. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11577-11585.	1.3	10
101	Electron-Pair Distribution in Chemical Bond Formation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1916-1923.	1.1	6
102	Aromaticity of acenes: the model of migrating π -circuits. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13430-13436.	1.3	36
103	Mechanism of the Selective Fe-Catalyzed Arene Carbon–Hydrogen Bond Functionalization. <i>ACS Catalysis</i> , 2018, 8, 4313-4322.	5.5	32
104	Influence of the charge on the reactivity of azafullerenes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28011-28018.	1.3	11
105	Aromaticity Determines the Relative Stability of Kinked vs. Straight Topologies in Polycyclic Aromatic Hydrocarbons. <i>Frontiers in Chemistry</i> , 2018, 6, 561.	1.8	41
106	Stereocontrolled Photoinduced Electron Transfer in Metal–Fullerene Hybrids. <i>Chemistry - A European Journal</i> , 2018, 24, 13020-13025.	1.7	17
107	Regioselectivity of the Pauson–Khand reaction in single-walled carbon nanotubes. <i>Nanoscale</i> , 2018, 10, 15078-15089.	2.8	11
108	Expedient Preparation of Open-Cage Fullerenes by Rhodium(I)-Catalyzed [2+2+2] Cycloaddition of Dienes and C ₆₀ : An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 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. <i>International Journal of Molecular Sciences</i> , 2018, 19, 1974.	1.8	14
110	The electronic structure and stability of germanium tubes $\text{Ge}_{30}\text{H}_{12}$ and $\text{Ge}_{33}\text{H}_{12}$. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23467-23479.	1.3	6
111	Expeditious Preparation of Open-Cage Fullerenes by Rhodium(I)-Catalyzed [2+2+2] Cycloaddition of Dienes and C_{60} : An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2018, 24, 10653-10661.	1.7	28
112	Tuning diastereoisomerism in platinum(II) phosphino- and aminothioloato hydrido complexes. <i>New Journal of Chemistry</i> , 2017, 41, 3015-3028.	1.4	1
113	Reactivity Patterns of (Protonated) Compound II and Compound I of Cytochrome P450: Which is the Better Oxidant?. <i>Chemistry - A European Journal</i> , 2017, 23, 6406-6418.	1.7	71
114	Is coronene better described by Clar's aromatic sextet model or by the AdNDP representation?. <i>Journal of Computational Chemistry</i> , 2017, 38, 1606-1611.	1.5	30
115	The role of the long-range exchange corrections in the description of electron delocalization in aromatic species. <i>Journal of Computational Chemistry</i> , 2017, 38, 1640-1654.	1.5	69
116	Understanding the Reactivity of Ion-Encapsulated Fullerenes. <i>Chemistry - A European Journal</i> , 2017, 23, 11030-11036.	1.7	33
117	Can Baird's and Clar's Rules Combined Explain Triplet State Energies of Polycyclic Conjugated Hydrocarbons with Fused $4n$ - and $(4n + 2)$ -Rings?. <i>Journal of Organic Chemistry</i> , 2017, 82, 6327-6340.	1.7	55
118	Mechanism of the Suzuki-Miyaura Cross-Coupling Reaction Mediated by $[\text{Pd}(\text{NHC})(\text{allyl})\text{Cl}]$ Precatalysts. <i>Organometallics</i> , 2017, 36, 2088-2095.	1.1	68
119	Rationalizing the relative abundances of trimetallic nitride template-based endohedral metallofullerenes from aromaticity measures. <i>Chemical Communications</i> , 2017, 53, 4140-4143.	2.2	5
120	Predicting and Understanding the Reactivity of Aza[60]fullerenes. <i>Journal of Organic Chemistry</i> , 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. <i>New Journal of Chemistry</i> , 2017, 41, 1168-1178.	1.4	9
122	The electron density of delocalized bonds (EDDB) applied for quantifying aromaticity. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 28970-28981.	1.3	114
123	A Computational Study of the Intermolecular [2+2+2] Cycloaddition of Acetylene and C_{60} Catalyzed by Wilkinson's Catalyst. <i>Chemistry - A European Journal</i> , 2017, 23, 15067-15072.	1.7	11
124	Does the endohedral borospherene supersalt $\text{FLi}_2@B_{39}$ maintain the superconducting properties of its subunits?. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21276-21281.	1.3	6
125	The key role of aromaticity in the structure and reactivity of C_{60} and endohedral metallofullerenes. <i>Inorganica Chimica Acta</i> , 2017, 468, 38-48.	1.2	8
126	Rhodium-Catalyzed [2+2+2] Cycloaddition Reactions of Linear Allene-Ynes to afford Fused Tricyclic Scaffolds: Insights into the Mechanism. <i>Chemistry - A European Journal</i> , 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. <i>Chemical Communications</i> , 2017, 53, 9922-9925.	2.2	15
128	Effect of incarcerated HF on the exohedral chemical reactivity of HF@C_{60} . <i>Chemical Communications</i> , 2017, 53, 10993-10996.	2.2	26
129	Why Aromaticity Is a Suspicious Concept? Why?. <i>Frontiers in Chemistry</i> , 2017, 5, 22.	1.8	108
130	Theoretical estimation of the rate of photoinduced charge transfer reactions in triphenylamine C_{60} donor-acceptor conjugate. <i>Journal of Computational Chemistry</i> , 2016, 37, 1396-1405.	1.5	10
131	Reactivity and Selectivity of Bowl-Shaped Polycyclic Aromatic Hydrocarbons: Relationship to C_{60} . <i>Chemistry - A European Journal</i> , 2016, 22, 1368-1378.	1.7	31
132	In Silico Olefin Metathesis with Ru-Based Catalysts Containing N-Heterocyclic Carbenes Bearing C_{60} Fullerenes. <i>Chemistry - A European Journal</i> , 2016, 22, 6617-6623.	1.7	15
133	Understanding the Reactivity of Planar Polycyclic Aromatic Hydrocarbons: Towards the Graphene Limit. <i>Chemistry - A European Journal</i> , 2016, 22, 10572-10580.	1.7	27
134	Photoinduced Charge Separation in the Carbon Nano-Onion $\text{C}_{60}@C_{240}$. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5798-5804.	1.1	10
135	Reaction Mechanism and Regioselectivity of the Bingel-Hirsch Addition of Dimethyl Bromomalonate to La@C_{20} . <i>Chemistry - A European Journal</i> , 2016, 22, 5953-5962.	1.7	23
136	The Regioselectivity of Bingel-Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. <i>Angewandte Chemie</i> , 2016, 128, 2420-2423.	1.6	9
137	Celebrating the 150th anniversary of the Kekulé benzene structure. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11587-11588.	1.3	26
138	Rules of Aromaticity. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2016, , 321-335.	0.6	7
139	Structural Preferences in Phosphanylthiolato Platinum(II) Complexes. <i>ChemistryOpen</i> , 2016, 5, 51-59.	0.9	6
140	Planar vs. three-dimensional X_6Y_4 , X_2Y_4 , and X_3Y_3 ($\text{X, Y = B, Tl, U, Q, O, P, r, g, B, T, O, v}$) Physical Chemistry Chemical Physics, 2016, 18, 21102-21110.	1.3	0
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