Maryam Koohi

List of Publications by Year
in descending order

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30	495	623734	794594
papers	citations	14	19
		h-index	g-index

30	30	30	218
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Estimating the stability and reactivity of cyclic tetrahalo substituted germylenes: A density functional theory investigation. Journal of Physical Organic Chemistry, 2020, 33, e4032.	1.9	14
2	A density functional theory perspective on 2,2,9,9â€tetrahalostannacyclononaâ€3,5,7â€trienylidenes. Journal of Physical Organic Chemistry, 2020, 33, e4031.	1.9	14
3	Substituted Hammick carbenes: The effects of fused rings and hetero atoms through DFT calculations. Journal of Physical Organic Chemistry, 2020, 33, e4023.	1.9	16
4	Structure, stability, MEP, NICS, reactivity, and NBO of Siâ€“Ge nanocages evolved from C20 fullerene at DFT. Monatshefte FÃ¼r Chemie, 2020, 151, 693-710.	1.8	14
5	Substituent effects on stability, MEP, NBO analysis, and reactivity of 2,2,9,9-tetrahalosilacyclonona-3,5,7-trienylidenes, at density functional theory. Monatshefte FÃ¼r Chemie, 2020, 151, 11-23.	1.8	23
6	Cyclononaâ€3,5,7â€trienylidene and its Si, Ge, Sn, and Pb analogs versus their Î±â€halogenated derivatives at B3LYP and MP2 methods. Journal of Physical Organic Chemistry, 2019, 32, e4013.	1.9	18
7	(E)â€3â€Xâ€indolineâ€2â€ones as potent and selective inhibitors against different receptor tyrosine kinase (RTKs) in solution vs gas phase, at DFT. Journal of Physical Organic Chemistry, 2019, 32, e3929.	1.9	4
8	Characterization of C₂₀ fullerene and its isolated C_{20â€“}<scp>_nG</scp>e_n derivatives (nÂ=Â1â€5) by alternating germanium atom(s) in equatorial position: A <scp>DFT</scp> survey. Heteroatom Chemistry, 2018, 29, .	0.7	15
9	Structure, stability, and electronic properties of AlP nanocages evolved from the world's smallest caged fullerene C 20 : A computational study at DFT. Journal of Molecular Structure, 2018, 1159, 118-134.	3.6	17
10	Novel X- and Y-substituted heterofullerenes X4Y4C12 developed from the nanocage C20, where Xâ€‰=â€‰B, Al, Ga, Si and Yâ€‰=â€‰N, P, As, Ge: a comparative investigation on their structural, stability, and electronic properties at DFT. Structural Chemistry, 2018, 29, 909-920.	2.0	21
11	Characterization of nonsegregated C₁₇Si₃ heterofullerenic isomers using density functional theory method. Journal of the Chinese Chemical Society, 2018, 65, 1453-1464.	1.4	16
12	Substituent effect on structure, stability, and aromaticity of novel <scp>B_nN_mC_{20â€“(n+m)}</scp> heterofullerenes. Journal of Physical Organic Chemistry, 2017, 30, e3682.	1.9	17
13	A comparative study on the Ge₆C₁₄heterofullerene nanocages: a density functional survey. Journal of Physical Organic Chemistry, 2017, 30, e3678.	1.9	13
14	Introducing boranorcaradienes with more stability than their corresponding borepins: Reversal of tautomerization via substituents at theoretical levels. Journal of Physical Organic Chemistry, 2017, 30, e3714.	1.9	3
15	Silicon impacts on structure, stability and aromaticity of C20-nSin heterofullerenes (nÂ=Â1â€“10): A density functional perspective. Journal of Molecular Structure, 2017, 1127, 522-531.	3.6	31
16	Characterizations of B and N heteroatoms as substitutional doping on structure, stability, and aromaticity of novel heterofullerenes evolved from the smallest fullerene cage C₂₀: a density functional theory perspective. Journal of Physical Organic Chemistry, 2016, 29, 514-522.	1.9	25
17	Computational Study of Solvent Effects on Characterizations of (E)â€3â€Xâ€indolineâ€2â€thiones Derivatives as Antivirus and Anticancer Compounds. Bulletin of the Korean Chemical Society, 2015, 36, 1985-1991.	1.9	4
18	Substituent effects on cyclononaâ€3,5,7â€trienylidenes: a quest for stable carbenes at density functional theory level. Journal of Physical Organic Chemistry, 2015, 28, 514-526.	1.9	25

#	Article	IF	Citations
19	C20â^'n Ge n heterofullerenes (nÂ=Â5â€“10) on focus: a density functional perspective. Monatshefte FÃ¼r Chemie, 2015, 146, 1409-1417.	1.8	16
20	Cyclacenes and short zigzag nanotubes with alternanting Geâ€•C bonds: theoretical impacts of Ge on the ground state, strain, and band gap. Journal of Physical Organic Chemistry, 2014, 27, 735-746.	1.9	18
21	Visible light photocatalytic activity of reduced graphene oxide synergistically enhanced by successive inclusion of Î³-Fe2O3, TiO2, and Ag nanoparticles. Materials Science in Semiconductor Processing, 2014, 26, 69-78.	4.0	31
22	Ylide stabilized carbenes: a computational study. Journal of Physical Organic Chemistry, 2014, 27, 902-908.	1.9	11
23	Breathing viability into cyclonona-3,5,7-trienylidenes via Î±-dimethyl and Î¬-moieties at DFT. Journal of Physical Organic Chemistry, 2013, 26, 540-550.	1.9	26
24	A selective nanocatalyst for an efficient Ugi reaction: Magnetically recoverable Cu(acac)2/NH2-T/SiO2@Fe3O4 nanoparticles. Journal of Chemical Sciences, 2013, 125, 1347-1357.	1.5	18
25	2,2,9,9â€Tetramethylcyclononaâ€3,5,7â€trienylidene vs. its heterocyclic analogues: A quest for stable carbenes at DFT. Journal of Physical Organic Chemistry, 2013, 26, 908-916.	1.9	25
26	Heteroatom impacts on structure, stability and aromaticity of XnC20â^'n fullerenes: A theoretical prediction. Computational and Theoretical Chemistry, 2010, 940, 19-28.	1.5	21
27	Umbrella inversions of cyclononatetraenylidenes at ab initio and DFT. Computational and Theoretical Chemistry, 2007, 810, 53-64.	1.5	8
28	Ring flips of allenes (C9H7X) over triplet carbenes at ab initio and DFT levels (X=H, F, Cl, Br). Computational and Theoretical Chemistry, 2007, 815, 21-29.	1.5	9
29	Transition state characteristics of planar singlet 2,4,6,8-cyclononatetraenylidenes and its halo derivatives, via ab initio. Computational and Theoretical Chemistry, 2005, 724, 61-71.	1.5	11
30	Mirror image conversions of cyclic conjugated non-planar allenes, C9H7X (X=H, F, Cl, Br). Computational and Theoretical Chemistry, 2005, 755, 91-98.	1.5	11