Miquel Sol

List of Publications by Citations

435 papers	17,020 citations	68 h-index	106 g-index
513 ext. papers	18,929 ext. citations	5.4 avg, IF	7.03 L-index

#	Paper	IF	Citations
435	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, 3911-47	68.1	580
434	The delocalization index as an electronic aromaticity criterion: application to a series of planar polycyclic aromatic hydrocarbons. *Chemistry - A European Journal*, **2003**, 9, 400-6	4.8	347
433	Theoretical Studies of Some Transition-Metal-Mediated Reactions of Industrial and Synthetic Importance. *Chemical Reviews*, **2000**, 100, 439-494	68.1	333
432	The aromatic fluctuation index (FLU): a new aromaticity index based on electron delocalization. *Journal of Chemical Physics*, **2005**, 122, 14109	3.9	321
431	Hydrogen-hydrogen bonding in planar biphenyl, predicted by atoms-in-molecules theory, does not exist. *Chemistry - A European Journal*, **2006**, 12, 2889-95	4.8	280
430	Quantifying aromaticity with electron delocalisation measures. *Chemical Society Reviews*, **2015**, 44, 6434-51	51.5	246
429	Forty years of Clar's aromatic sextet rule. *Frontiers in Chemistry*, **2013**, 1, 22	5	236
428	On the performance of some aromaticity indices: a critical assessment using a test set. *Journal of Computational Chemistry*, **2008**, 29, 1543-54	3.5	222
427	Nucleophilic aryl fluorination and aryl halide exchange mediated by a Cu(I)/Cu(III) catalytic cycle. *Journal of the American Chemical Society*, **2011**, 133, 19386-92	16.4	200
426	A model of the chemical bond must be rooted in quantum mechanics, provide insight, and possess predictive power. *Chemistry - A European Journal*, **2006**, 12, 2902-5	4.8	191
425	Aromaticity and three-dimensional aromaticity: two sides of the same coin?. *Angewandte Chemie - International Edition*, **2014**, 53, 12191-5	16.4	187
424	Chemical bonding in transition metal carbene complexes. *Journal of Organometallic Chemistry*, **2005**, 690, 6178-6204	2.3	180
423	Electron sharing indexes at the correlated level. Application to aromaticity calculations. *Faraday Discussions*, **2007**, 135, 325-45; discussion 367-401, 503-6	3.6	178
422	Polycyclic benzenoids: why kinked is more stable than straight. *Journal of Organic Chemistry*, **2007**, 72, 1134-42	4.2	177
421	Local aromaticity of [n]acenes, [n]phenacenes, and [n]helicenes (n = 1-9). *Journal of Organic Chemistry*, **2005**, 70, 2509-21	4.2	168
420	The calculation of electron localization and delocalization indices at the Hartree–Fock, density functional and post-Hartree–Fock levels of theory. *Theoretical Chemistry Accounts*, **2002**, 107, 362-371	1.9	166
419	Relation between the substituent effect and aromaticity. *Journal of Organic Chemistry*, **2004**, 69, 6634-40	4.2	163

418	Electron-pairing analysis from localization and delocalization indices in the framework of the atoms-in-molecules theory. *Theoretical Chemistry Accounts*, **2002**, 108, 214-224	1.9	155
417	Nucleus-independent chemical shift (NICS) profiles in a series of monocyclic planar inorganic compounds. *Journal of Organometallic Chemistry*, **2006**, 691, 4359-4366	2.3	133
416	Assessment of Clar's aromatic sextet rule by means of PDI, NICS and HOMA indicators of local aromaticity. *Journal of Physical Organic Chemistry*, **2005**, 18, 785-791	2.1	131
415	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	23.2	124
414	On the validity of the maximum hardness principle and the minimum electrophilicity principle during chemical reactions. *Journal of Physical Chemistry A*, **2013**, 117, 1843-52	2.8	121
413	Ab initio and DFT benchmark study for nucleophilic substitution at carbon (SN2@C) and silicon (SN2@Si). *Journal of Computational Chemistry*, **2005**, 26, 1497-504	3.5	120
412	Facile C-H bond cleavage via a proton-coupled electron transfer involving a C-H...Cu(II) interaction. *Journal of the American Chemical Society*, **2010**, 132, 12299-306	16.4	119
411	The reactivity of endohedral fullerenes. What can be learnt from computational studies?. *Physical Chemistry Chemical Physics*, **2011**, 13, 3585-603	3.6	117
410	Comparison of the AIM delocalization index and the Mayer and fuzzy atom bond orders. *Journal of Physical Chemistry A*, **2005**, 109, 9904-10	2.8	117
409	Importance of the basis set for the spin-state energetics of iron complexes. *Journal of Physical Chemistry A*, **2008**, 112, 6384-91	2.8	115
408	An insight into the local aromaticities of polycyclic aromatic hydrocarbons and fullerenes. *Chemistry - A European Journal*, **2003**, 9, 1113-22	4.8	113
407	Electron localization function at the correlated level. *Journal of Chemical Physics*, **2006**, 125, 24301	3.9	112
406	Dispersion corrections essential for the study of chemical reactivity in fullerenes. *Journal of Physical Chemistry A*, **2011**, 115, 3491-6	2.8	108
405	Analysis of solvent effects on the Menshutkin reaction. *Journal of the American Chemical Society*, **1991**, 113, 2873-2879	16.4	108
404	A new all-round density functional based on spin states and S(N)2 barriers. *Journal of Chemical Physics*, **2009**, 131, 094103	3.9	104
403	Properties of aromaticity indices based on the one-electron density matrix. *Journal of Physical Chemistry A*, **2007**, 111, 6521-5	2.8	104
402	Interplay between intramolecular resonance-assisted hydrogen bonding and aromaticity in o-hydroxyaryl aldehydes. *Journal of Organic Chemistry*, **2006**, 71, 5241-8	4.2	104
401	Electron delocalization and aromaticity in low-lying excited states of archetypal organic compounds. *Physical Chemistry Chemical Physics*, **2011**, 13, 20690-703	3.6	102

400	Basis set and electron correlation effects on ab initio electronic and vibrational nonlinear optical properties of conjugated organic molecules. *Journal of Chemical Physics*, **2003**, 118, 711-718	3.9	102
399	Density Functional Study of the [2+2]- and [2+3]-Cycloaddition Mechanisms for the Osmium-Catalyzed Dihydroxylation of Olefins. *Organometallics*, **1997**, 16, 13-19	3.8	101
398	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. *Journal of Chemical Theory and Computation*, **2010**, 6, 2736-42	6.4	99
397	Local aromaticity of the six-membered rings in pyracylene. A difficult case for the NICS indicator of aromaticity. *Journal of Organic Chemistry*, **2004**, 69, 7537-42	4.2	99
396	A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity. *Symmetry*, **2010**, 2, 1156-1179	2.7	98
395	On the validity of the maximum hardness and minimum polarizability principles for nontotally symmetric vibrations. *Journal of the American Chemical Society*, **2001**, 123, 7951-2	16.4	98
394	Fine-tuning the electronic properties of highly stable organometallic Cu(III) complexes containing monoanionic macrocyclic ligands. *Chemistry - A European Journal*, **2005**, 11, 5146-56	4.8	97
393	Aromaticity of distorted benzene rings: exploring the validity of different indicators of aromaticity. *Journal of Physical Chemistry A*, **2007**, 111, 4513-21	2.8	94
392	Metalloaromaticity. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 105-122	7.9	93
391	Discrepancy between common local aromaticity measures in a series of carbazole derivatives. *Physical Chemistry Chemical Physics*, **2004**, 6, 314-318	3.6	92
390	Why do cycloaddition reactions involving C60 prefer [6,6] over [5,6] bonds?. *Chemistry - A European Journal*, **2013**, 19, 7416-22	4.8	88
389	Molecular structure and bonding of copper cluster monocarbonyls CunCO (n = 1-9). *Journal of Physical Chemistry B*, **2006**, 110, 6526-36	3.4	88
388	Energy landscapes of nucleophilic substitution reactions: a comparison of density functional theory and coupled cluster methods. *Journal of Computational Chemistry*, **2007**, 28, 1551-1560	3.5	87
387	Hückel's Rule of Aromaticity Categorizes Aromatic closo Boron Hydride Clusters. *Chemistry - A European Journal*, **2016**, 22, 7437-43	4.8	84
386	The role of aromaticity in determining the molecular structure and reactivity of (endohedral metallo)fullerenes. *Chemical Society Reviews*, **2014**, 43, 5089-105	58.5	84
385	Six questions on topology in theoretical chemistry. *Computational and Theoretical Chemistry*, **2015**, 1053, 2-16	2	81
384	Ground and Low-Lying States of Cu2+□2O. A Difficult Case for Density Functional Methods. *Journal of Physical Chemistry A*, **2004**, 108, 6072-6078	2.8	79
383	Mechanism of the addition reaction of alkyl azides to [60]fullerene and the subsequent N2 extrusion to form monoimino-[60]fullerenes. *Journal of Organic Chemistry*, **2001**, 66, 433-42	4.2	79

382	Why Aromaticity Is a Suspicious Concept? Why?. *Frontiers in Chemistry*, **2017**, 5, 22	5	76
381	E2 and SN2 Reactions of X(-) + CH3CH2X (X = F, Cl); an ab Initio and DFT Benchmark Study. *Journal of Chemical Theory and Computation*, **2008**, 4, 929-40	6.4	76
380	. *Journal of Physical Chemistry A*, **1999**, 103, 4525-4532	2.8	74
379	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	6.4	73
378	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	6.4	71
377	Modeling the structure-property relationships of nanoneedles: A journey toward nanomedicine. *Journal of Computational Chemistry*, **2009**, 30, 275-84	3.5	71
376	Molecular Structure and Bond Characterization of the Fischer-Type Chromium□Carbene Complexes (CO)5CrC(X)R (X = H, OH, OCH3, NH2, NHCH3 and R = H, CH3, CHCH2, Ph, C?CH). *Organometallics*, **2002**, 21, 4182-4191	3.8	71
375	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.5	70
374	Chemical reactivity of D3h C78 (metallo)fullerene: regioselectivity changes induced by Sc3N encapsulation. *Journal of the American Chemical Society*, **2008**, 130, 6206-14	16.4	70
373	Too Persistent to Give Up: Aromaticity in Boron Clusters Survives Radical Structural Changes. *Journal of the American Chemical Society*, **2020**, 142, 9396-9407	16.4	70
372	The Diels-Alder reaction on endohedral Y3N@C78: the importance of the fullerene strain energy. *Journal of the American Chemical Society*, **2009**, 131, 129-39	16.4	69
371	On the electron-pair nature of the hydrogen bond in the framework of the atoms in molecules theory. *Chemical Physics Letters*, **2003**, 369, 248-255	2.5	69
370	Excited-State Intramolecular Proton Transfer and Rotamerism of 2-(2□hydroxyvinyl)benzimidazole and 2-(2□hydroxyphenyl)imidazole. *Journal of Physical Chemistry A*, **1999**, 103, 4413-4420	2.8	69
369	Are the maximum hardness and minimum polarizability principles always obeyed in nontotally symmetric vibrations?. *Journal of Chemical Physics*, **2002**, 117, 10561-10570	3.9	67
368	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, 9982-92	3.9	66
367	Electronic and Vibrational Nonlinear Optical Properties of Five Representative Electrides. *Journal of Chemical Theory and Computation*, **2012**, 8, 2688-97	6.4	64
366	Oxidative addition of the ethane C-C bond to Pd. An ab initio benchmark and DFT validation study. *Journal of Computational Chemistry*, **2005**, 26, 1006-20	3.5	63
365	Interplay between intramolecular resonance-assisted hydrogen bonding and local aromaticity. II. 1,3-Dihydroxyaryl-2-aldehydes. *Journal of Organic Chemistry*, **2009**, 74, 2059-66	4.2	62

364	A trinuclear Pt(II) compound with short Pt-Pt-Pt contacts. An analysis of the influence of pi-pi stacking interactions on the strength and length of the Pt-Pt bond. *Dalton Transactions*, **2006**, 1188-96	4.3	62
363	Foundations and recent developments on molecular quantum similarity. *Topics in Current Chemistry* , **1995**, 31-62		62
362	Density Functional Study of the [2+2+2] Cyclotrimerization of Acetylene Catalyzed by Wilkinson's Catalyst, RhCl(PPh3)3. *Organometallics*, **2010**, 29, 562-569	3.8	60
361	Local aromaticity of the lowest-lying singlet States of [N]acenes (N = 6-9). *Journal of Physical Chemistry A*, **2005**, 109, 10629-32	2.8	60
360	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, 5108-13	2.8	60
359	A theoretical study of steric and electronic effects in the rhodium-catalyzed carbonylation reactions. *Journal of the American Chemical Society*, **2001**, 123, 12294-302	16.4	60
358	Diels-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, 9721-6	2.8	59
357	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	16.4	59
356	New Solids Based on B12N12 Fullerenes. *Journal of Physical Chemistry C*, **2007**, 111, 13354-13360	3.8	58
355	Basis set and electron correlation effects on initial convergence for vibrational nonlinear optical properties of conjugated organic molecules. *Journal of Chemical Physics*, **2004**, 120, 6346-55	3.9	58
354	Aromaticity and Three-Dimensional Aromaticity: Two sides of the Same Coin?. *Angewandte Chemie*, **2014**, 126, 12387-12391	3.6	56
353	Copper(II) hexaaza macrocyclic binuclear complexes obtained from the reaction of their copper(I) derivates and molecular dioxygen. *Inorganic Chemistry*, **2006**, 45, 3569-81	5.1	56
352	Reactivity Patterns of (Protonated) Compound II and Compound I of Cytochrome P450: Which is the Better Oxidant?. *Chemistry - A European Journal*, **2017**, 23, 6406-6418	4.8	55
351	On the mechanism of the thermal retrocycloaddition of pyrrolidinofullerenes (retro-Prato reaction). *Chemistry - A European Journal*, **2008**, 14, 5198-206	4.8	55
350	The Hammond Postulate and the Principle of Maximum Hardness in Some Intramolecular Rearrangement Reactions. *Journal of Physical Chemistry A*, **1999**, 103, 8847-8852	2.8	55
349	Complete mechanism of sigma* intramolecular aromatic hydroxylation through O2 activation by a macrocyclic dicopper(I) complex. *Journal of the American Chemical Society*, **2008**, 130, 17710-7	16.4	54
348	Mechanism of the Suzuki–Miyaura Cross-Coupling Reaction Mediated by [Pd(NHC)(allyl)Cl] Precatalysts. *Organometallics*, **2017**, 36, 2088-2095	3.8	53
347	On the existence and characterization of molecular electrides. *Chemical Communications*, **2015**, 51, 4865-88	5.8	53

346	Aromaticity and electronic delocalization in all-metal clusters with single, double, and triple aromatic character. *Theoretical Chemistry Accounts*, **2011**, 128, 419-431	1.9	53
345	The electron density of delocalized bonds (EDDB) applied for quantifying aromaticity. *Physical Chemistry Chemical Physics*, **2017**, 19, 28970-28981	3.6	52
344	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, 1700-2	4.2	52
343	Regioselective intramolecular Pauson-Khand reactions of C60: an electrochemical study and theoretical underpinning. *Chemistry - A European Journal*, **2005**, 11, 2716-29	4.8	52
342	Theoretical Study of Diels−Alder Cycloadditions of Butadiene to C70. An Insight into the Chemical Reactivity of C70 as Compared to C60. *The Journal of Physical Chemistry*, **1996**, 100, 7449-7454		51
341	Local aromaticity in natural nucleobases and their size-expanded benzo-fused derivatives. *Journal of Physical Chemistry A*, **2006**, 110, 12249-58	2.8	51
340	Mechanism of the Manganese-Pincer-Catalyzed Acceptorless Dehydrogenative Coupling of Nitriles and Alcohols. *Journal of the American Chemical Society*, **2019**, 141, 2398-2403	16.4	50
339	A dissected ring current model for assessing magnetic aromaticity: a general approach for both organic and inorganic rings. *Journal of Computational Chemistry*, **2011**, 32, 2422-31	3.5	50
338	Reaction Mechanisms for Graphene and Carbon Nanotube Fluorination. *Journal of Physical Chemistry C*, **2010**, 114, 3340-3345	3.8	50
337	Thermal [2+2] intramolecular cycloadditions of fuller-1,6-enynes. *Angewandte Chemie - International Edition*, **2006**, 45, 1439-42	16.4	50
336	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	3.8	49
335	Mechanistic Studies of Transition-Metal-Catalyzed [2 + 2 + 2] Cycloaddition Reactions. *Chemical Reviews*, **2021**, 121, 1894-1979	68.1	49
334	Maximum aromaticity as a guiding principle for the most suitable hosting cages in endohedral metallofullerenes. *Angewandte Chemie - International Edition*, **2013**, 52, 9275-8	16.4	48
333	Acidic C-H Bond as a Proton Donor in Excited State Intramolecular Proton Transfer Reactions. *Journal of Chemical Theory and Computation*, **2015**, 11, 1046-54	6.4	48
332	Mechanistic insights into the chemistry of RuII complexes containing Cl and DMSO ligands. *Inorganic Chemistry*, **2007**, 46, 10707-16	5.1	48
331	Theoretical Study on Acetaldehyde and Ethanol Elimination from the Hydrogenation of CH3(O)CCo(CO)3. *Organometallics*, **1996**, 15, 2611-2618	3.8	48
330	Theoretical investigation of the relative stabilities of XSSX and X2SS isomers (X = F, Cl, H, and CH3). *Journal of Computational Chemistry*, **1995**, 16, 465-477	3.5	48
329	The role of the long-range exchange corrections in the description of electron delocalization in aromatic species. *Journal of Computational Chemistry*, **2017**, 38, 1640-1654	3.5	47

328	The exohedral Diels-Alder reactivity of the titanium carbide endohedral metallofullerene Ti2C2@D(3h)-C78: comparison with D(3h)-C78 and M3N@D(3h)-C78 (M=Sc and Y) reactivity. *Chemistry - A European Journal*, **2012**, 18, 7141-54	4.8	47
327	Molecular Size and Pyramidalization: Two Keys for Understanding the Reactivity of Fullerenes. *The Journal of Physical Chemistry*, **1995**, 99, 10752-10758		47
326	Full exploration of the Diels-Alder cycloaddition on metallofullerenes M3N@C80 (M = Sc, Lu, Gd): the D(5h) versus I(h) isomer and the influence of the metal cluster. *Chemistry - A European Journal*, **2012**, 18, 8944-56	4.8	46
325	An analysis of the changes in aromaticity and planarity along the reaction path of the simplest Diels□Alder reaction. Exploring the validity of different indicators of aromaticity. *Computational and Theoretical Chemistry*, **2005**, 727, 165-171		45
324	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	3.6	45
323	Computational methods to predict the reactivity of nanoparticles through structure-property relationships. *Expert Opinion on Drug Delivery*, **2010**, 7, 295-305	8	44
322	On the quality of the hardness kernel and the Fukui function to evaluate the global hardness. *Journal of Computational Chemistry*, **2007**, 28, 574-83	3.5	44
321	Electron delocalization and aromaticity measures within the H□kel molecular orbital method. *Computational and Theoretical Chemistry*, **2007**, 811, 3-11		44
320	Aromaticity analysis of lithium cation/pi complexes of aromatic systems. *ChemPhysChem*, **2005**, 6, 2552-61	3.2	44
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318	Covalency in Highly Polar Bonds. Structure and Bonding of Methylalkalimetal Oligomers (CH3M)n (M = Li-Rb; n = 1, 4). *Journal of Chemical Theory and Computation*, **2006**, 2, 965-80	6.4	43
317	A comparative analysis by means of quantum molecular similarity measures of density distributions derived from conventional ab initio and density functional methods. *Journal of Chemical Physics*, **1996**, 104, 636-647	3.9	43
316	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	16.4	43
315	Cyclo[18]carbon: the smallest all-carbon electron acceptor. *Chemical Communications*, **2020**, 56, 352-355	5.8	43
314	Understanding the reactivity of endohedral metallofullerenes: C78 versus Sc3N@C78. *Chemistry - A European Journal*, **2015**, 21, 5760-8	4.8	42
313	The missing entry in the agostic-anagostic series: Rh(I)-□(1)-C interactions in P(CH)P pincer complexes. *Inorganic Chemistry*, **2015**, 54, 2960-9	5.1	42
312	Rhodium(I)-catalysed intramolecular [2+2+2] cyclotrimerisations of 15-, 20- and 25-membered azamacrocycles: experimental and theoretical mechanistic studies. *Chemistry - A European Journal*, **2009**, 15, 5289-300	4.8	42
311	Reactivity and regioselectivity of noble gas endohedral fullerenes Ng@C(60) and Ng(2)@C(60) (Ng=He-Xe). *Chemistry - A European Journal*, **2009**, 15, 13111-23	4.8	42

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306	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, 8913-21	4.2	40
305	Analysis of the effects of N-substituents on some aspects of the aromaticity of imidazoles and pyrazoles. *Journal of Physical Chemistry A*, **2011**, 115, 8571-7	2.8	40
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301	Spin-state-corrected Gaussian-type orbital basis sets. *Journal of Physical Chemistry A*, **2010**, 114, 7191-7	2.8	39
300	Molecular mechanism of acid-triggered aryl-halide reductive elimination in well-defined aryl-Cu(III)-halide species. *Dalton Transactions*, **2010**, 39, 10458-63	4.3	39
299	On the mechanism of action of fullerene derivatives in superoxide dismutation. *Chemistry - A European Journal*, **2010**, 16, 3207-14	4.8	39
298	Spin-state splittings of iron(II) complexes with trispyrazolyl ligands. *Polyhedron*, **2010**, 29, 84-93	2.7	39
297	Fast O2 binding at dicopper complexes containing Schiff-base dinucleating ligands. *Inorganic Chemistry*, **2007**, 46, 4997-5012	5.1	39
296	Regiospecific C-H bond activation: reversible H/D exchange promoted by CuI complexes with triazamacrocyclic ligands. *Angewandte Chemie - International Edition*, **2006**, 45, 2941-4	16.4	39
295	Can Baird's and Clar's Rules Combined Explain Triplet State Energies of Polycyclic Conjugated Hydrocarbons with Fused 4n□and (4n + 2)□Rings?. *Journal of Organic Chemistry*, **2017**, 82, 6327-6340	4.2	38
294	Electrochemical control of the regioselectivity in the exohedral functionalization of C60: the role of aromaticity. *Chemical Communications*, **2013**, 49, 1220-2	5.8	38
293	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	3.8	37

292	A complete guide on the influence of metal clusters in the Diels-Alder regioselectivity of I(h)-C80 endohedral metallofullerenes. *Chemistry - A European Journal*, **2013**, 19, 14931-40	4.8	36
291	Theoretical Study on the Thermodynamics of the Elimination of Formic Acid in the Last Step of the Hydrogenation of CO2 Catalyzed by Rhodium Complexes in the Gas Phase and Supercritical CO2. *Organometallics*, **1998**, 17, 3164-3168	3.8	36
290	The linear response kernel of conceptual DFT as a measure of aromaticity. *Physical Chemistry Chemical Physics*, **2012**, 14, 3960-7	3.6	35
289	Examining the planarity of poly(3,4-ethylenedioxythiophene): consideration of self-rigidification, electronic, and geometric effects. *Journal of Physical Chemistry A*, **2010**, 114, 1023-8	2.8	35
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285	Performance of 3D-space-based atoms-in-molecules methods for electronic delocalization aromaticity indices. *Journal of Computational Chemistry*, **2011**, 32, 386-95	3.5	33
284	H-bond-assisted regioselective (cis-1) intramolecular nucleophilic addition of the hydroxyl group to [60]fullerene. *Journal of Organic Chemistry*, **2009**, 74, 1480-7	4.2	33
283	Analysis of H□kel's [4n + 2] rule through electronic delocalization measures. *Journal of Physical Chemistry A*, **2008**, 112, 13231-8	2.8	33
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281	Origin of Reactivity Trends of Noble Gas Endohedral Fullerenes Ng2@C60 (Ng = He to Xe). *Journal of Chemical Theory and Computation*, **2014**, 10, 3863-70	6.4	32
280	Enantiospecific cis-trans isomerization in chiral fulleropyrrolidines: hydrogen-bonding assistance in the carbanion stabilization in H2O@C60. *Journal of the American Chemical Society*, **2015**, 137, 1190-7	16.4	32
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