Miquel Sol

List of Publications by Year in Descending Order

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	Path-dependency of energy decomposition analysis & the elusive nature of bonding.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	4
434	Three-Dimensional Fully π-Conjugated Macrocycles: When 3D-Aromatic and When 2D-Aromatic-in-3D?. *Journal of the American Chemical Society*, **2022**,	16.4	6
433	Fast and Simple Evaluation of the Catalysis and Selectivity Induced by External Electric Fields. *ACS Catalysis*, **2021**, 11, 14467-14479	13.1	3
432	Photoinduced electron transfer in non-covalent complexes of C60 and phosphangulene oxide derivatives. *Dalton Transactions*, **2021**, 50, 16214-16222	4.3	0
431	Cage···Cage Interaction: Boron Cluster-Based Noncovalent Bond and Its Applications in Solid-State Materials. *Jacs Au*, **2021**, 1, 2047-2057		0
430	The Relative Stability of Indole Isomers Is a Consequence of the Glidewell-Lloyd Rule. *Journal of Physical Chemistry A*, **2021**, 125, 230-234	2.8	5
429	Guidelines for Tuning the Excited State Hückel–Baird Hybrid Aromatic Character of Pro-Aromatic Quinoidal Compounds**. *Angewandte Chemie*, **2021**, 133, 10343-10353	3.6	2
428	Guidelines for Tuning the Excited State Hückel-Baird Hybrid Aromatic Character of Pro-Aromatic Quinoidal Compounds*. *Angewandte Chemie - International Edition*, **2021**, 60, 10255-10265	16.4	9
427	Efficient synthesis of amine-functionalized graphene oxide by ultrasound-assisted reactions and density functional theory mechanistic insight. *Applied Nanoscience (Switzerland)*, **2021**, 11, 1637-1649	3.3	0
426	How Do Defects in Carbon Nanostructures Regulate the Photoinduced Electron Transfer Processes? The Case of Phenine Nanotubes. *ChemPhysChem*, **2021**, 22, 1178-1186	3.2	3
425	(Invited) Water-soluble fullerenes (C60 and C70) with photoinduced ROS generation. *ECS Meeting Abstracts*, **2021**, MA2021-01, 618-618	0	
424	Double-Carrousel Mechanism for Mn-Catalyzed Dehydrogenative Amide Synthesis from Alcohols and Amines. *ACS Catalysis*, **2021**, 11, 6155-6161	13.1	6
423	Fluxional bis(phenoxy-imine) Zr and Ti catalysts for polymerization. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	
422	[10]CPP-Based Inclusion Complexes of Charged Fulleropyrrolidines. Effect of the Charge Location on the Photoinduced Electron Transfer. *Chemistry - A European Journal*, **2021**, 27, 8737-8744	4.8	2
421	Synthesis of Fused Dihydroazepine Derivatives of Fullerenes by a Rh-Catalyzed Cascade Process. *Advanced Synthesis and Catalysis*, **2021**, 363, 3835-3844	5.6	3
420	Chelation enforcing a dual gold configuration in the catalytic hydroxyphenoxylation of alkynes. *Applied Organometallic Chemistry*, **2021**, 35, e6362	3.1	3
419	Mechanistic Studies of Transition-Metal-Catalyzed [2 + 2 + 2] Cycloaddition Reactions. *Chemical Reviews*, **2021**, 121, 1894-1979	68.1	49

418	Aromaticity of nucleic acid bases. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1509	7.9	1
417	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	5.2	17
416	Aromaticity Survival in Hydrofullerenes: The Case of C H with Its Aromatic Circuits. *Chemistry - A European Journal*, **2021**, 27, 802-808	4.8	2
415	An unprecedented electronic circuit involving an odd number of carbon atoms in a grossly warped non-planar nanographene. *Chemical Communications*, **2021**, 57, 3087-3090	5.8	5
414	Photoinduced electron transfer in nano-Saturn complexes of fullerene. *Physical Chemistry Chemical Physics*, **2021**, 23, 2126-2133	3.6	1
413	Acenes and phenacenes in their lowest-lying triplet states. Does kinked remain more stable than straight?. *Physical Chemistry Chemical Physics*, **2021**, 23, 13574-13582	3.6	4
412	Photoinduced electron transfer in mechanically interlocked suit[3]ane systems. *Journal of Materials Chemistry C*, **2021**, 9, 9436-9445	7.1	3
411	The electron density of delocalized bonds (EDDBs) as a measure of local and global aromaticity **2021**, 259-284		4
410	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	1.9	2
409	Unexpected Disparity in Photoinduced Reactions of C and C in Water with the Generation of O or O. *Jacs Au*, **2021**, 1, 1601-1611		1
408	Evaluation of charge-transfer rates in fullerene-based donor-acceptor dyads with different density functional approximations. *Physical Chemistry Chemical Physics*, **2021**, 23, 5376-5384	3.6	3
407	Analysis of the electronic delocalization in some isoelectronic analogues of B doped with beryllium and/or carbon. *Physical Chemistry Chemical Physics*, **2020**, 22, 12245-12259	3.6	6
406	Triquinoline- versus Fullerene-Based Cycloparaphenylene Ionic Complexes: Comparison of Photoinduced Charge-Shift Reactions. *Chemistry - A European Journal*, **2020**, 26, 10896-10902	4.8	4
405	Substituted adenine quartets: interplay between substituent effect, hydrogen bonding, and aromaticity.. *RSC Advances*, **2020**, 10, 23350-23358	3.7	3
404	Mechanism of the Facile Nitrous Oxide Fixation by Homogeneous Ruthenium Hydride Pincer Catalysts. *Inorganic Chemistry*, **2020**, 59, 9374-9383	5.1	8
403	Probing the Origin of Adaptive Aromaticity in 16-Valence-Electron Metallapentalenes. *Chemistry - A European Journal*, **2020**, 26, 12964-12971	4.8	12
402	Effect of Alkali Metal Cations on Length and Strength of Hydrogen Bonds in DNA Base Pairs. *ChemPhysChem*, **2020**, 21, 2112-2126	3.2	8
401	The nido-Cage??? Bond: A Non-covalent Interaction between Boron Clusters and Aromatic Rings and Its Applications. *Angewandte Chemie*, **2020**, 132, 9103-9110	3.6	4

400	The nido-Cage???Bond: A Non-covalent Interaction between Boron Clusters and Aromatic Rings and Its Applications. *Angewandte Chemie - International Edition*, **2020**, 59, 9018-9025	16.4	15
399	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	2.8	2
398	Cyclo[18]carbon: the smallest all-carbon electron acceptor. *Chemical Communications*, **2020**, 56, 352-355	5.8	43
397	Do Carbon Nano-onions Behave as Nanoscopic Faraday Cages? A Comparison of the Reactivity of C , C , C @C , Li @C , Li @C , and Li @C @C. *Chemistry - A European Journal*, **2020**, 26, 804-808	4.8	7
396	The influence of the pH on the reaction mechanism of water oxidation by a Ru(bda) catalyst. *Catalysis Today*, **2020**, 358, 278-283	5.3	7
395	Iodane-Guided ortho CH Allylation. *Angewandte Chemie*, **2020**, 132, 20376-20382	3.6	2
394	Bingel-Hirsch Addition of Diethyl Bromomalonate to Ion-Encapsulated Fullerenes M@C (M=Li, Na, K, Mg, Ca, and Cl). *Chemistry - A European Journal*, **2020**, 26, 14481-14487	4.8	2
393	Iodane-Guided ortho C-H Allylation. *Angewandte Chemie - International Edition*, **2020**, 59, 20201-20207	16.4	2
392	Probing the Origin of Adaptive Aromaticity in 16-Valence-Electron Metallapentalenes. *Chemistry - A European Journal*, **2020**, 26, 12902	4.8	
391	Understanding the performance of a bisphosphonate Ru water oxidation catalyst. *Dalton Transactions*, **2020**, 49, 14052-14060	4.3	8
390	All-metal Baird aromaticity. *Chemical Communications*, **2020**, 56, 12522-12525	5.8	14
389	Photoinduced electron transfer in nanotube?C inclusion complexes: phenine . nanographene nanotubes. *Chemical Communications*, **2020**, 56, 12624-12627	5.8	4
388	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	3.4	4
387	Covalent Functionalization of Single-Walled Carbon Nanotubes by the Bingel Reaction for Building Charge-Transfer Complexes. *Journal of Organic Chemistry*, **2020**, 85, 11721-11731	4.2	5
386	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
385	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
384	Hypsochromic solvent shift of the charge separation band in ionic donor-acceptor Li@C?[10]CPP. *Chemical Communications*, **2019**, 55, 11195-11198	5.8	11
383	Exploiting the Aromatic Chameleon Character of Fulvenes for Computational Design of Baird-Aromatic Triplet Ground State Compounds. *Chemistry - an Asian Journal*, **2019**, 14, 1870-1878	4.5	8

382	Regioselectivity in Diels-Alder Cycloadditions of C Fullerene with a Triplet Ground State. *Journal of Organic Chemistry*, **2019**, 84, 9017-9024	4.2	6
381	Photoinduced Charge Shift in Li+-Doped Giant Nested Fullerenes. *Journal of Physical Chemistry C*, **2019**, 123, 16525-16532	3.8	6
380	Effect of Exocyclic Substituents and π-System Length on the Electronic Structure of Chichibabin Diradical(oid)s. *ACS Omega*, **2019**, 4, 10845-10853	3.9	6
379	Innenrücktitelbild: All-Fullerene Electron Donor–Acceptor Conjugates (Angew. Chem. 21/2019). *Angewandte Chemie*, **2019**, 131, 7217-7217	3.6	1
378	All-Fullerene Electron Donor-Acceptor Conjugates. *Angewandte Chemie - International Edition*, **2019**, 58, 6932-6937	16.4	19
377	Is Excited-State Aromaticity a Driving Force for Planarization of Dibenzannelated 8π-Electron Heterocycles?. *ChemPlusChem*, **2019**, 84, 712-721	2.8	23
376	All-Fullerene Electron Donor–Acceptor Conjugates. *Angewandte Chemie*, **2019**, 131, 7006-7011	3.6	8
375	Electron Delocalization in Planar Metallacycles: Hückel or Möbius Aromatic?. *ChemistryOpen*, **2019**, 8, 219-227	2.3	27
374	The Coulomb Hole of the Ne Atom. *ChemistryOpen*, **2019**, 8, 411-417	2.3	4
373	Open-shell jellium aromaticity in metal clusters. *Chemical Communications*, **2019**, 55, 5559-5562	5.8	9
372	Decomposition of the electronic activity in competing [5,6] and [6,6] cycloaddition reactions between C and cyclopentadiene. *Physical Chemistry Chemical Physics*, **2019**, 21, 5039-5048	3.6	7
371	A Rh-Catalyzed Cycloisomerization/Diels-Alder Cascade Reaction of 1,5-Bisallenes for the Synthesis of Polycyclic Heterocycles. *Organic Letters*, **2019**, 21, 6608-6613	6.2	12
370	Examining the Factors That Govern the Regioselectivity in Rhodium-Catalyzed Alkyne Cyclotrimerization. *Organometallics*, **2019**, 38, 2853-2862	3.8	19
369	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.3	70
368	Photoinduced electron transfer and unusual environmental effects in fullerene-Zn-porphyrin-BODIPY triads. *Physical Chemistry Chemical Physics*, **2019**, 21, 25098-25107	3.6	17
367	Tuning the Strength of the Resonance-Assisted Hydrogen Bond in Acenes and Phenacenes with Two -Hydroxyaldehyde Groups-The Importance of Topology. *Journal of Organic Chemistry*, **2019**, 84, 15538-15548	4.2	6
366	Connecting and combining rules of aromaticity. Towards a unified theory of aromaticity. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1404	7.9	19
365	Peculiar Photoinduced Electron Transfer in Porphyrin-Fullerene Akamptisomers. *Chemistry - A European Journal*, **2019**, 25, 2577-2585	4.8	7

364	Rationalizing the Regioselectivity of the Diels-Alder Biscycloaddition of Fullerenes. *Journal of Organic Chemistry*, **2018**, 83, 3285-3292	4.2	10
363	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. *Chemistry - A European Journal*, **2018**, 24, 9853-9859	4.8	18
362	Reliable charge assessment on encapsulated fragment for endohedral systems. *Scientific Reports*, **2018**, 8, 2882	4.9	3
361	Tuning the Strength of the Resonance-Assisted Hydrogen Bond in o-Hydroxybenzaldehyde by Substitution in the Aromatic Ring. *Journal of Physical Chemistry A*, **2018**, 122, 2279-2287	2.8	19
360	On the regioselectivity of the Diels-Alder cycloaddition to C in high spin states. *Physical Chemistry Chemical Physics*, **2018**, 20, 11577-11585	3.6	6
359	Electron-Pair Distribution in Chemical Bond Formation. *Journal of Physical Chemistry A*, **2018**, 122, 1916-1923	2.8	4
358	Aromaticity of acenes: the model of migrating □-circuits. *Physical Chemistry Chemical Physics*, **2018**, 20, 13430-13436	3.6	17
357	Mechanism of the Selective Fe-Catalyzed Arene Carbon□Hydrogen Bond Functionalization. *ACS Catalysis*, **2018**, 8, 4313-4322	13.1	23
356	Regioselectivity of the Pauson-Khand reaction in single-walled carbon nanotubes. *Nanoscale*, **2018**, 10, 15078-15089	7.7	6
355	Expeditious Preparation of Open-Cage Fullerenes by Rhodium(I)-Catalyzed [2+2+2] Cycloaddition of Diynes and C60: An Experimental and Theoretical Study. *Chemistry - A European Journal*, **2018**, 24, 10561-10561	4.8	
354	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,	6.3	13
353	The electronic structure and stability of germanium tubes GeH and GeH. *Physical Chemistry Chemical Physics*, **2018**, 20, 23467-23479	3.6	5
352	Expeditious Preparation of Open-Cage Fullerenes by Rhodium(I)-Catalyzed [2+2+2] Cycloaddition of Diynes and C : An Experimental and Theoretical Study. *Chemistry - A European Journal*, **2018**, 24, 10653-10661	4.8	19
351	Influence of the charge on the reactivity of azafullerenes. *Physical Chemistry Chemical Physics*, **2018**, 20, 28011-28018	3.6	10
350	Aromaticity Determines the Relative Stability of Kinked vs. Straight Topologies in Polycyclic Aromatic Hydrocarbons. *Frontiers in Chemistry*, **2018**, 6, 561	5	20
349	Stereocontrolled Photoinduced Electron Transfer in Metal-Fullerene Hybrids. *Chemistry - A European Journal*, **2018**, 24, 13020-13025	4.8	14
348	Tuning diastereoisomerism in platinum(II) phosphino- and aminothiolato hydrido complexes. *New Journal of Chemistry*, **2017**, 41, 3015-3028	3.6	1
347	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

346	Is coronene better described by Clar's aromatic sextet model or by the AdNDP representation?. *Journal of Computational Chemistry*, **2017**, 38, 1606-1611	3.5	19
345	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
344	Understanding the Reactivity of Ion-Encapsulated Fullerenes. *Chemistry - A European Journal*, **2017**, 23, 11030-11036	4.8	28
343	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
342	Mechanism of the Suzuki Miyaura Cross-Coupling Reaction Mediated by [Pd(NHC)(allyl)Cl] Precatalysts. *Organometallics*, **2017**, 36, 2088-2095	3.8	53
341	Rationalizing the relative abundances of trimetallic nitride template-based endohedral metallofullerenes from aromaticity measures. *Chemical Communications*, **2017**, 53, 4140-4143	5.8	5
340	Predicting and Understanding the Reactivity of Aza[60]fullerenes. *Journal of Organic Chemistry*, **2017**, 82, 754-758	4.2	18
339	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	3.6	6
338	The electron density of delocalized bonds (EDDB) applied for quantifying aromaticity. *Physical Chemistry Chemical Physics*, **2017**, 19, 28970-28981	3.6	52
337	A Computational Study of the Intermolecular [2+2+2] Cycloaddition of Acetylene and C Catalyzed by Wilkinson's Catalyst. *Chemistry - A European Journal*, **2017**, 23, 15067-15072	4.8	7
336	Does the endohedral borospherene supersalt FLi@B maintain the "super" properties of its subunits?. *Physical Chemistry Chemical Physics*, **2017**, 19, 21276-21281	3.6	6
335	The key role of aromaticity in the structure and reactivity of C60 and endohedral metallofullerenes. *Inorganica Chimica Acta*, **2017**, 468, 38-48	2.7	6
334	Rhodium-Catalyzed [2+2+2] Cycloaddition Reactions of Linear Allene-Ene-Ynes to afford Fused Tricyclic Scaffolds: Insights into the Mechanism. *Chemistry - A European Journal*, **2017**, 23, 14889-14899	4.8	13
333	Unusual reactivity of rhodium carbenes with allenes: an efficient asymmetric synthesis of methylenetetrahydropyran scaffolds. *Chemical Communications*, **2017**, 53, 9922-9925	5.8	7
332	Effect of incarcerated HF on the exohedral chemical reactivity of HF@C. *Chemical Communications*, **2017**, 53, 10993-10996	5.8	17
331	Why Aromaticity Is a Suspicious Concept? Why?. *Frontiers in Chemistry*, **2017**, 5, 22	5	76
330	Planar vs. three-dimensional X6(2-), X2Y4(2-), and X3Y3(2-) (X, Y = B, Al, Ga) metal clusters: an analysis of their relative energies through the turn-upside-down approach. *Physical Chemistry Chemical Physics*, **2016**, 18, 21102-10	3.6	6
329	The Driving Force of Photoinduced Charge Separation in Metal-Cluster-Encapsulated Triphenylamine-[80]fullerenes. *Chemistry - A European Journal*, **2016**, 22, 17305-17310	4.8	5

328	Exploring the validity of the Glidewell–Lloyd extension of Clar's sextet rule: assessment from polycyclic conjugated hydrocarbons. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	16
327	The Regioselectivity of Bingel-Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. *Angewandte Chemie - International Edition*, **2016**, 55, 2374-7	16.4	28
326	Analysis of a Compound Class with Triplet States Stabilized by Potentially Baird Aromatic [10]Annulenyl Dicationic Rings. *Chemistry - A European Journal*, **2016**, 22, 2793-800	4.8	25
325	Hückel's Rule of Aromaticity Categorizes Aromatic closo Boron Hydride Clusters. *Chemistry - A European Journal*, **2016**, 22, 7437-43	4.8	84
324	Complexes of adamantane-based group 13 Lewis acids and superacids: Bonding analysis and thermodynamics of hydrogen splitting. *Journal of Computational Chemistry*, **2016**, 37, 1355-62	3.5	7
323	Fmoc-RGDS based fibrils: atomistic details of their hierarchical assembly. *Physical Chemistry Chemical Physics*, **2016**, 18, 1265-78	3.6	13
322	Octahedral aromaticity in (2S+1)A1g X6(q) clusters (X = Li-C and Be-Si, S = 0-3, and q = -2 to +4). *Physical Chemistry Chemical Physics*, **2016**, 18, 11700-6	3.6	10
321	Bonding description of the Harpoon mechanism. This paper is dedicated to Andreas Savin on the occasion of his 65th birthday.View all notes. *Molecular Physics*, **2016**, 114, 1345-1355	1.7	11
320	Structural Preferences in Phosphanylthiolato Platinum(II) Complexes. *ChemistryOpen*, **2016**, 5, 2	2.3	1
319	(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	3.8	26
318	Nitrite to nitric oxide interconversion by heme FeII complex assisted by [CuI(tmpa)]+. *Structural Chemistry*, **2016**, 27, 409-417	1.8	3
317	Theoretical estimation of the rate of photoinduced charge transfer reactions in triphenylamine C60 donor-acceptor conjugate. *Journal of Computational Chemistry*, **2016**, 37, 1396-405	3.5	8
316	Reactivity and Selectivity of Bowl-Shaped Polycyclic Aromatic Hydrocarbons: Relationship to C60. *Chemistry - A European Journal*, **2016**, 22, 1368-78	4.8	31
315	In Silico Olefin Metathesis with Ru-Based Catalysts Containing N-Heterocyclic Carbenes Bearing C60 Fullerenes. *Chemistry - A European Journal*, **2016**, 22, 6617-23	4.8	9
314	Understanding the Reactivity of Planar Polycyclic Aromatic Hydrocarbons: Towards the Graphene Limit. *Chemistry - A European Journal*, **2016**, 22, 10572-80	4.8	24
313	Photoinduced Charge Separation in the Carbon Nano-Onion C60@C240. *Journal of Physical Chemistry A*, **2016**, 120, 5798-804	2.8	10
312	Reaction Mechanism and Regioselectivity of the Bingel-Hirsch Addition of Dimethyl Bromomalonate to La@C2v -C82. *Chemistry - A European Journal*, **2016**, 22, 5953-62	4.8	18
311	The Regioselectivity of Bingel–Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. *Angewandte Chemie*, **2016**, 128, 2420-2423	3.6	7

310	Rules of Aromaticity. *Challenges and Advances in Computational Chemistry and Physics*, **2016**, 321-335	0.7	5
309	Structural Preferences in Phosphanylthiolato Platinum(II) Complexes. *ChemistryOpen*, **2016**, 5, 51-9	2.3	5
308	On the existence and characterization of molecular electrides. *Chemical Communications*, **2015**, 51, 4865-8	6.8	53
307	Understanding the reactivity of endohedral metallofullerenes: C78 versus Sc3N@C78. *Chemistry - A European Journal*, **2015**, 21, 5760-8	4.8	42
306	The missing entry in the agostic-anagostic series: Rh(I)-η(1)-C interactions in P(CH)P pincer complexes. *Inorganic Chemistry*, **2015**, 54, 2960-9	5.1	42
305	Why 1,2-quinone derivatives are more stable than their 2,3-analogues?. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	13
304	Quantifying aromaticity with electron delocalisation measures. *Chemical Society Reviews*, **2015**, 44, 6434-51	5.15	246
303	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, 8223-36	5.1	21
302	Reusable manganese compounds containing pyrazole-based ligands for olefin epoxidation reactions. *Dalton Transactions*, **2015**, 44, 17529-43	4.3	17
301	A theoretical study of the aromaticity in neutral and anionic borole compounds. *Dalton Transactions* , **2015**, 44, 6740-7	4.3	34
300	Six questions on topology in theoretical chemistry. *Computational and Theoretical Chemistry*, **2015**, 1053, 2-16	2	81
299	Enantioselective Rhodium(I) Donor Carbenoid-Mediated Cascade Triggered by a Base-Free Decomposition of Arylsulfonyl Hydrazones. *Chemistry - A European Journal*, **2015**, 21, 16240-5	4.8	31
298	On the Reaction Mechanism of the Rhodium-Catalyzed Arylation of Fullerene (C60) with Organoboron Compounds in the Presence of Water. *ChemistryOpen*, **2015**, 4, 774-8	2.3	10
297	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
296	Extent of charge separation and exciton delocalization for electronically excited states in a triphenylamine-C60 donor–acceptor conjugate: a combined molecular dynamics and TD-DFT study. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	12
295	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
294	Three-center bonding analyzed from correlated and uncorrelated third-order reduced density matrices. *Computational and Theoretical Chemistry*, **2015**, 1053, 173-179	2	8
293	Understanding the Exohedral Functionalization of Endohedral Metallofullerenes. *Carbon Materials*, **2015**, 67-99		

292	Exploring the potential energy surface of E$_{12}$ clusters (E=Group 13 element): the quest for inverse carbon-free sandwiches. *Chemistry - A European Journal*, **2014**, 20, 4583-90	4.8	17
291	Stereoselective rhodium-catalysed [2+2+2] cycloaddition of linear allene-ene/yne-allene substrates: reactivity and theoretical mechanistic studies. *Chemistry - A European Journal*, **2014**, 20, 5034-45	4.8	30
290	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
289	A new mild synthetic route to N-arylated pyridazinones from aryldiazonium salts. *Chemical Communications*, **2014**, 50, 8073-6	5.8	4
288	σ-aromaticity and three-dimensional aromaticity: two sides of the same coin?. *Angewandte Chemie - International Edition*, **2014**, 53, 12191-5	16.4	187
287	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	3.8	7
286	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
285	Electroactive polymers for the detection of morphine. *Journal of Polymer Research*, **2014**, 21, 1	2.7	6
284	Aromaticity and Magnetic Properties of 1- and 2-Indenones and Their Aza Derivatives. *European Journal of Organic Chemistry*, **2014**, 2014, 5370-5377	3.2	4
283	Analysis of the Aromaticity of Five-Membered Heterometallacycles Containing Os, Ru, Rh, and Ir. *Organometallics*, **2014**, 33, 1762-1773	3.8	25
282	New Approximation to the Third-Order Density. Application to the Calculation of Correlated Multicenter Indices. *Journal of Chemical Theory and Computation*, **2014**, 10, 3055-65	6.4	29
281	Dinuclear Ru-aqua complexes for selective epoxidation catalysis based on supramolecular substrate orientation effects. *Chemistry - A European Journal*, **2014**, 20, 3898-902	4.8	28
280	Aromaticity of Organic and Inorganic Heterocycles. *Topics in Heterocyclic Chemistry*, **2014**, 129-160	0.2	0
279	σ-Aromaticity and Three-Dimensional Aromaticity: Two sides of the Same Coin?. *Angewandte Chemie*, **2014**, 126, 12387-12391	3.6	56
278	Computational insight into Wilkinson's complex catalyzed [2 + 2 + 2] cycloaddition mechanism leading to pyridine formation. *Journal of Organometallic Chemistry*, **2014**, 768, 15-22	2.3	12
277	Aromatic properties of 8-hydroxyquinoline and its metal complexes. *Open Chemistry*, **2013**, 11, 655-663	1.6	6
276	Aromaticity as the driving force for the stability of non-IPR endohedral metallofullerene Bingel-Hirsch adducts. *Chemical Communications*, **2013**, 49, 8767-9	5.8	21
275	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

274	Comparison between alkalimetal and group 11 transition metal halide and hydride tetramers: molecular structure and bonding. *Journal of Physical Chemistry A*, **2013**, 117, 8026-34	2.8	9
273	Unraveling the origin of the relative stabilities of group 14 M2N2(2+) (M, N = C, Si, Ge, Sn, and Pb) isomer clusters. *Journal of Physical Chemistry A*, **2013**, 117, 10462-9	2.8	12
272	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	2.5	5
271	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, 2458-65	5.1	11
270	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
269	Analysis of the Relative Stabilities of Ortho, Meta, and Para MClY(XC4H4)(PH3)2Heterometallabenzenes (M = Rh, Ir; X = N, P; Y = Cl and M = Ru, Os; X = N, P; Y = CO). *Organometallics*, **2013**, 32, 4892-4903	3.8	26
268	Examining the formation of specific interactions between poly(3,4-ethylenedioxythiophene) and nucleotide bases. *RSC Advances*, **2013**, 3, 2639	3.7	5
267	Electrochemical control of the regioselectivity in the exohedral functionalization of C60: the role of aromaticity. *Chemical Communications*, **2013**, 49, 1220-2	5.8	38
266	Metalloaromaticity. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 105-122	7.9	93
265	Diels-Alder and retro-Diels-Alder cycloadditions of (1,2,3,4,5-pentamethyl)cyclopentadiene to La@C(2v)-C(82): regioselectivity and product stability. *Chemistry - A European Journal*, **2013**, 19, 4468-79	4.8	25
264	A simple link between hydrocarbon and borohydride chemistries. *Chemistry - A European Journal*, **2013**, 19, 4169-75	4.8	33
263	Why do cycloaddition reactions involving C60 prefer [6,6] over [5,6] bonds?. *Chemistry - A European Journal*, **2013**, 19, 7416-22	4.8	88
262	Ruthenium complexes with chiral bis-pinene ligands: an array of subtle structural diversity. *Inorganic Chemistry*, **2013**, 52, 4985-92	5.1	7
261	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	1.7	4
260	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
259	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, 520-32	6.4	9
258	N-Tetradentate SPANamine Derivatives and Their MnII-Complexes as Catalysts for Epoxidation of Alkenes. *European Journal of Inorganic Chemistry*, **2013**, 2013, 1213-1224	2.3	19
257	Maximum Aromaticity as a Guiding Principle for the Most Suitable Hosting Cages in Endohedral Metallofullerenes. *Angewandte Chemie*, **2013**, 125, 9445-9448	3.6	8

256	Forty years of Clar's aromatic sextet rule. *Frontiers in Chemistry*, **2013**, 1, 22	5	236
255	Complete intramolecular aromatic hydroxylation mechanism through O2 activation by a Schiff base macrocyclic dicopper(I) complex. *Beilstein Journal of Organic Chemistry*, **2013**, 9, 585-93	2.5	6
254	Molecular structures of M2N2(2-) (M and N = B, Al, and Ga) clusters using the gradient embedded genetic algorithm. *Physical Chemistry Chemical Physics*, **2012**, 14, 14850-9	3.6	17
253	On the electronic structure of second generation HoveydaGrubbs alkene metathesis precursors. *Computational and Theoretical Chemistry*, **2012**, 996, 57-67	2	20
252	Product formation in the Prato reaction on Sc3N@D(5h)-C80: preference for [5,6]-bonds, and not pyracylenic bonds. *Chemical Communications*, **2012**, 48, 2486-8	5.8	26
251	Properties of poly(3-halidethiophene)s. *Physical Chemistry Chemical Physics*, **2012**, 14, 10050-62	3.6	7
250	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, 1671-83	6.4	18
249	Direct detection of key intermediates in rhodium(I)-catalyzed [2+2+2] cycloadditions of alkynes by ESI-MS. *Chemistry - A European Journal*, **2012**, 18, 13097-107	4.8	32
248	The linear response kernel of conceptual DFT as a measure of aromaticity. *Physical Chemistry Chemical Physics*, **2012**, 14, 3960-7	3.6	35
247	Electronic and Vibrational Nonlinear Optical Properties of Five Representative Electrides. *Journal of Chemical Theory and Computation*, **2012**, 8, 2688-97	6.4	64
246	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
245	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
244	Tuning the electronic properties by width and length modifications of narrow- diameter carbon nanotubes for nanomedicine. *Current Medicinal Chemistry*, **2012**, 19, 5219-25	4.3	15
243	All-metal aromatic clusters M4(2-) (M = B, Al, and Ga). Are electrons distortive or not?. *Physical Chemistry Chemical Physics*, **2011**, 13, 20673-81	3.6	11
242	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
241	Understanding conjugation and hyperconjugation from electronic delocalization measures. *Journal of Physical Chemistry A*, **2011**, 115, 13104-13	2.8	25
240	The reactivity of endohedral fullerenes. What can be learnt from computational studies?. *Physical Chemistry Chemical Physics*, **2011**, 13, 3585-603	3.6	117
239	Routes of electron delocalization in 4-substituted-1,2-benzoquinones. *Journal of Organic Chemistry*, **2011**, 76, 550-6	4.2	12

238	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
237	Dispersion corrections essential for the study of chemical reactivity in fullerenes. *Journal of Physical Chemistry A*, **2011**, 115, 3491-6	2.8	108
236	Binding of 6-mer single-stranded homo-nucleotides to poly(3,4-ethylenedioxythiophene): specific hydrogen bonds with guanine. *Soft Matter*, **2011**, 7, 9922	3.6	13
235	Organomagnesium clusters: Structure, stability, and bonding in archetypal models. *Journal of Organometallic Chemistry*, **2011**, 696, 4104-4111	2.3	12
234	Ab initio design of chelating ligands relevant to Alzheimer's disease: influence of metalloaromaticity. *Journal of Physical Chemistry A*, **2011**, 115, 12659-66	2.8	17
233	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
232	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
231	Electron delocalization and aromaticity in low-lying excited states of archetypal organic compounds. *Physical Chemistry Chemical Physics*, **2011**, 13, 20690-703	3.6	102
230	A multi-scale approach to spin crossover in Fe(II) compounds. *Physical Chemistry Chemical Physics*, **2011**, 13, 10449-56	3.6	17
229	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
228	Measuring electron sharing between atoms in first-principle simulations. *Theoretical Chemistry Accounts*, **2011**, 130, 27-36	1.9	5
227	Theoretical studies on aromaticity of selected hydroxypyrones. Part 3#. Chelatoaromaticity phenomenon in metalcomplexes of hydroxypyrones. *Journal of Physical Organic Chemistry*, **2011**, 24, 499-506	2.1	14
226	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
225	Inter- and intramolecular dispersion interactions. *Journal of Computational Chemistry*, **2011**, 32, 1117-27	3.5	32
224	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
223	Intramolecular [2+2+2] cycloaddition reactions of yne-ene-yne and yne-yne-ene enediynes catalysed by Rh(I): experimental and theoretical mechanistic studies. *Chemistry - A European Journal*, **2011**, 17, 14493-507	4.8	25
222	Open-shell spherical aromaticity: the 2N2 + 2N + 1 (with S = N + □) rule. *Chemical Communications*, **2011**, 47, 11647-9	5.8	40
221	A donor-functionalized, silyl-substituted pentadienyllithium: structural insight from experiment and theory. *Chemical Communications*, **2011**, 47, 6162-4	5.8	13

220	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. *Journal of Chemical Theory and Computation*, **2011**, 7, 1231	6.4	7
219	Nuclear shieldings with the SSB-D functional. *Journal of Physical Chemistry A*, **2011**, 115, 1250-6	2.8	16
218	RhCl(PPh3)3-Catalyzed Intramolecular Cycloaddition of Enediynes: The Nature of the Tether and Substituents Controls the Reaction Mechanism. *Organometallics*, **2011**, 30, 3151-3159	3.8	19
217	New ru(II) complexes containing oxazoline ligands as epoxidation catalysts. Influence of the substituents on the catalytic performance. *Inorganic Chemistry*, **2011**, 50, 6044-54	5.1	26
216	The Chemical Reactivity of Fullerenes and Endohedral Fullerenes: A Theoretical Perspective. *Carbon Materials*, **2011**, 57-78		2
215	A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity. *Symmetry*, **2010**, 2, 1156-1179	2.7	98
214	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
213	Computational methods to predict the reactivity of nanoparticles through structure-property relationships. *Expert Opinion on Drug Delivery*, **2010**, 7, 295-305	8	44
212	Mechanism of the aminolysis of Fischer alkoxy and thiocarbene complexes: a DFT study. *Journal of Organic Chemistry*, **2010**, 75, 5821-36	4.2	18
211	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. *Journal of Chemical Theory and Computation*, **2010**, 6, 2736-42	6.4	99
210	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
209	Density Functional Calculations of E2 and SN2 Reactions: Effects of the Choice of Method, Algorithm, and Numerical Accuracy. *Journal of Chemical Theory and Computation*, **2010**, 6, 3145-52	6.4	26
208	Influence of confinement on hydrogen bond energy. The case of the FH□□NCH dimer. *Journal of Physical Chemistry A*, **2010**, 114, 10253-60	2.8	30
207	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
206	Reaction Mechanisms for Graphene and Carbon Nanotube Fluorination. *Journal of Physical Chemistry C*, **2010**, 114, 3340-3345	3.8	50
205	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
204	Spin-state-corrected Gaussian-type orbital basis sets. *Journal of Physical Chemistry A*, **2010**, 114, 7191-7	2.8	39
203	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

202	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
201	Ene reactions between two alkynes? Doors open to thermally induced cycloisomerization of macrocyclic triynes and enediynes. *Chemical Communications*, **2010**, 46, 2944-6	5.8	20
200	Accurate Description of Spin States and its Implications for Catalysis **2010**, 551-583		10
199	Patterns of pi-electron delocalization in aromatic and antiaromatic organic compounds in the light of H□kel's 4n + 2 rule. *Physical Chemistry Chemical Physics*, **2010**, 12, 7126-37	3.6	32
198	On the mechanism of action of fullerene derivatives in superoxide dismutation. *Chemistry - A European Journal*, **2010**, 16, 3207-14	4.8	39
197	Reactivity and Regioselectivity of Noble Gas Endohedral Fullerenes Ng@C60 and Ng2@C60 (Ng=He□e). *Chemistry - A European Journal*, **2010**, 16, 3878-3878	4.8	5
196	Spin-state splittings of iron(II) complexes with trispyrazolyl ligands. *Polyhedron*, **2010**, 29, 84-93	2.7	39
195	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
194	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
193	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
192	D□z benzannulation reactions: heteroatom and substituent effects in chromium Fischer carbene complexes. *Chemistry - A European Journal*, **2009**, 15, 12503-20	4.8	19
191	Homolytic versus heterolytic dissociation of alkalimetal halides: the effect of microsolvation. *ChemPhysChem*, **2009**, 10, 2955-65	3.2	13
190	Alkali Metal Complexes of Silyl-Substituted ansa-(Tris)allyl Ligands: Metal-, Co-Ligand- and Substituent-Dependent Stereochemistry. *European Journal of Inorganic Chemistry*, **2009**, 2009, 4157-4167	2.3	15
189	On the Regioselective Intramolecular Nucleophilic Addition of Thiols to C60. *European Journal of Organic Chemistry*, **2009**, 2009, 6231-6238	3.2	15
188	Modeling the structure-property relationships of nanoneedles: A journey toward nanomedicine. *Journal of Computational Chemistry*, **2009**, 30, 275-84	3.5	71
187	Tuning aromaticity in trigonal alkaline earth metal clusters and their alkali metal salts. *Journal of Computational Chemistry*, **2009**, 30, 2764-76	3.5	42
186	Theoretical study of the hydroxylation of phenolates by the Cu(2)O (2)(N,N'-dimethylethylenediamine) (2) (2+) complex. *Journal of Biological Inorganic Chemistry*, **2009**, 14, 229-42	3.7	16
185	Theoretical study of the hydroxylation of phenols mediated by an end-on bound superoxo-copper(II) complex. *Journal of Biological Inorganic Chemistry*, **2009**, 14, 273-85	3.7	11

184	Excess charge delocalization in organic and biological molecules: some theoretical notions. *Theoretical Chemistry Accounts*, **2009**, 123, 29-40	1.9	8
183	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
182	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
181	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
180	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, 1308-17	2.8	16
179	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
178	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
177	Competitive retro-cycloaddition reaction in fullerene dimers connected through pyrrolidinopyrazolino rings. *Journal of Organic Chemistry*, **2009**, 74, 8174-80	4.2	25
176	Regioselective intramolecular nucleophilic addition of alcohols to C60: one-step formation of a cis-1 bicyclic-fused fullerene. *Journal of Organic Chemistry*, **2009**, 74, 6253-9	4.2	30
175	Chemical bonding and aromaticity in metalloporphyrins,. *Canadian Journal of Chemistry*, **2009**, 87, 1063-1073	1.09	27
174	Local aromaticity of pristine and fluorinated carbon nanotubes. *Journal of Nanoscience and Nanotechnology*, **2009**, 9, 6078-83	1.3	8
173	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
172	Analysis of Hückel's [4n + 2] rule through electronic delocalization measures. *Journal of Physical Chemistry A*, **2008**, 112, 13231-8	2.8	33
171	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
170	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
169	New ruthenium(II) complexes with enantiomerically pure bis- and tris(pinene)-fused tridentate ligands. Synthesis, characterization and stereoisomeric analysis. *Inorganic Chemistry*, **2008**, 47, 8016-24	5.1	15
168	Coordination and haptotropic migration of Cr(CO)3 in polycyclic aromatic hydrocarbons: the effect of the size and the curvature of the substrate. *Journal of Physical Chemistry A*, **2008**, 112, 1202-13	2.8	31
167	Intramolecular Haptotropic Rearrangements of the Tricarbonylchromium Complex in Small Polycyclic Aromatic Hydrocarbons. *Organometallics*, **2008**, 27, 5230-5240	3.8	30

166	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
165	On the mechanism of the thermal retrocycloaddition of pyrrolidinofullerenes (retro-Prato reaction). *Chemistry - A European Journal*, **2008**, 14, 5198-206	4.8	55
164	The hardness kernel as the basis for global and local reactivity indices. *Journal of Computational Chemistry*, **2008**, 29, 1064-72	3.5	27
163	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
162	Mechanistic theoretical insight of Ru(II) catalysts with a meridional□facial bpea fashion competition. *Chemical Physics Letters*, **2008**, 458, 200-204	2.5	10
161	Coordination of bis(tricarbonylchromium) complexes to small polycyclic aromatic hydrocarbons: Structure, relative stabilities, and bonding. *Chemical Physics Letters*, **2008**, 465, 181-189	2.5	7
160	Nanosized trigonal prismatic and antiprismatic CuII coordination cages based on tricarboxylate linkers. *Dalton Transactions*, **2008**, 1679-82	4.3	10
159	Highly polar bonds and the meaning of covalency and ionicity--structure and bonding of alkali metal hydride oligomers. *Faraday Discussions*, **2007**, 135, 451-68; discussion 489-506	3.6	16
158	Theoretical study of the reaction mechanisms involved in the thermal intramolecular reactions of 1,6-fullerenynes. *Journal of Physical Chemistry A*, **2007**, 111, 5253-8	2.8	12
157	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
156	Didehydrophenanthrenes: structure, singlet-triplet splitting, and aromaticity. *Journal of Physical Chemistry A*, **2007**, 111, 5063-70	2.8	30
155	Table salt and other alkali metal chloride oligomers: structure, stability, and bonding. *Inorganic Chemistry*, **2007**, 46, 5411-8	5.1	17
154	Fast O2 binding at dicopper complexes containing Schiff-base dinucleating ligands. *Inorganic Chemistry*, **2007**, 46, 4997-5012	5.1	39
153	Properties of aromaticity indices based on the one-electron density matrix. *Journal of Physical Chemistry A*, **2007**, 111, 6521-5	2.8	104
152	Polycyclic benzenoids: why kinked is more stable than straight. *Journal of Organic Chemistry*, **2007**, 72, 1134-42	4.2	177
151	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
150	Covalent versus ionic bonding in alkalimetal fluoride oligomers. *Journal of Computational Chemistry* , **2007**, 28, 238-50	3.5	14
149	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

148	Electron delocalization and aromaticity measures within the Hückel molecular orbital method. *Computational and Theoretical Chemistry*, **2007**, 811, 3-11		44
147	Aromaticity changes along the reaction coordinate connecting the cyclobutadiene dimer to cubane and the benzene dimer to hexaprismane. *Structural Chemistry*, **2007**, 18, 773-783	1.8	13
146	The proton transfer reaction in malonaldehyde derivatives: Substituent effects and quasi-aromaticity of the proton bridge. *Chemical Physics*, **2007**, 342, 43-54	2.3	41
145	Chapter 3 The breakdown of the maximum hardness and minimum polarizability principles for nontotally symmetric vibrations. *Theoretical and Computational Chemistry*, **2007**, 31-45		2
144	Chapter 10 Electronic structure and reactivity of aromatic metal clusters. *Theoretical and Computational Chemistry*, **2007**, 19, 203-218		
143	Mechanistic insights into the chemistry of RuII complexes containing Cl and DMSO ligands. *Inorganic Chemistry*, **2007**, 46, 10707-16	5.1	48
142	New Solids Based on B12N12 Fullerenes. *Journal of Physical Chemistry C*, **2007**, 111, 13354-13360	3.8	58
141	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
140	Atropisomeric discrimination in new Ru(II) complexes containing the C(2)-symmetric didentate chiral phenyl-1,2-bisoxazolinic ligand. *Chemistry - A European Journal*, **2006**, 12, 2798-807	4.8	30
139	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
138	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
137	Thermal [2+2] intramolecular cycloadditions of fuller-1,6-enynes. *Angewandte Chemie - International Edition*, **2006**, 45, 1439-42	16.4	50
136	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
135	Electron fluctuation in pericyclic and pseudopericyclic reactions. *ChemPhysChem*, **2006**, 7, 111-3	3.2	42
134	Thermal [2+2] Intramolecular Cycloadditions of Fuller-1,6-enynes. *Angewandte Chemie*, **2006**, 118, 1467-1470	3.6	12
133	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
132	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
131	Pseudo-Jahn-Teller effect as the origin of the exalted frequency of the b2u Kekulé mode in the 1(1)B2u excited state of benzene. *Journal of Physical Chemistry A*, **2006**, 110, 11219-22	2.8	21

130	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
129	Local aromaticity in natural nucleobases and their size-expanded benzo-fused derivatives. *Journal of Physical Chemistry A*, **2006**, 110, 12249-58	2.8	51
128	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
127	Interplay between intramolecular resonance-assisted hydrogen bonding and aromaticity in o-hydroxyaryl aldehydes. *Journal of Organic Chemistry*, **2006**, 71, 5241-8	4.2	104
126	A Novel Exploration of the Hartree□Fock Homolytic Bond Dissociation Problem in the Hydrogen Molecule by Means of Electron Localization Measures. *Journal of Chemical Education*, **2006**, 83, 1243	2.4	19
125	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, 8901-11	2.8	6
124	New Ru complexes containing the N-tridentate bpea and phosphine ligands: consequences of meridional vs facial geometry. *Inorganic Chemistry*, **2006**, 45, 10520-9	5.1	40
123	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
122	Redox-controlled molecular flipper based on a chiral Cu complex. *Inorganic Chemistry*, **2006**, 45, 9643-5	5.1	9
121	Bonding in methylalkalimetals (CH(3)M)(n) (M = Li, Na, K; n = 1, 4). Agreement and divergences between AIM and ELF analyses. *Journal of Physical Chemistry B*, **2006**, 110, 7189-98	3.4	32
120	Electron localization function at the correlated level. *Journal of Chemical Physics*, **2006**, 125, 24301	3.9	112
119	Intramolecular ene reaction of 1,6-fullerenynes: a new synthesis of allenes. *Organic Letters*, **2006**, 8, 5959-62	5.2	30
118	O2 chemistry of dicopper complexes with alkyltriamine ligands. Comparing synergistic effects on O2 binding. *Inorganic Chemistry*, **2006**, 45, 5239-41	5.1	23
117	Molecular structure and bonding of copper cluster monocarbonyls CunCO (n = 1-9). *Journal of Physical Chemistry B*, **2006**, 110, 6526-36	3.4	88
116	Are nucleus-independent (NICS) and 1H NMR chemical shifts good indicators of aromaticity in □stacked polyfluorenes?. *Chemical Physics Letters*, **2006**, 428, 191-195	2.5	32
115	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
114	Analysis of electron delocalization in aromatic systems: individual molecular orbital contributions to para-delocalization indexes (PDI). *Journal of Physical Chemistry A*, **2006**, 110, 11569-74	2.8	25
113	Structure and bonding of methyl alkali metal molecules. *Journal of Molecular Modeling*, **2006**, 12, 563-8	2	8

112	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		27
111	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
110	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
109	Hydrogen bonding and aromaticity in the guanine□ytosine base pair interacting with metal cations (M = Cu+, Ca2+ and Cu2+). *Molecular Physics*, **2005**, 103, 163-173	1.7	23
108	Generalizing the breakdown of the maximum hardness and minimum polarizabilities principles for nontotally symmetric vibrations to non-pi-conjugated organic molecules. *Journal of Physical Chemistry A*, **2005**, 109, 615-21	2.8	20
107	Comment on the "Nature of bonding in the thermal cyclization of (Z)-1,2,4,6-heptatetraene and its heterosubstituted analogues". *Journal of Physical Chemistry B*, **2005**, 109, 7591-3; discussion 7594-5	3.4	16
106	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
105	Diastereoselective synthesis of fulleropyrrolidines from suitably functionalized chiral cyclobutanes. *Journal of Organic Chemistry*, **2005**, 70, 6929-32	4.2	22
104	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, 3256-62	4.2	33
103	Chemical bonding in transition metal carbene complexes. *Journal of Organometallic Chemistry*, **2005**, 690, 6178-6204	2.3	180
102	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
101	Local aromaticity of [n]acenes, [n]phenacenes, and [n]helicenes (n = 1-9). *Journal of Organic Chemistry*, **2005**, 70, 2509-21	4.2	168
100	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
99	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
98	Aromaticity analysis of lithium cation/pi complexes of aromatic systems. *ChemPhysChem*, **2005**, 6, 2552-61	3.2	44
97	Regioselective intramolecular Pauson-Khand reactions of C60: an electrochemical study and theoretical underpinning. *Chemistry - A European Journal*, **2005**, 11, 2716-29	4.8	52
96	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
95	The breakdown of the minimum polarizability principle in vibrational motions as an indicator of the most aromatic center. *Chemistry - A European Journal*, **2005**, 11, 6024-31	4.8	13

94	Basis set effects on the energy and hardness profiles of the hydrogen fluoride dimer. *Journal of Chemical Sciences*, **2005**, 117, 549-554	1.8	4
93	Ab initio and DFT modeling of stereoselective deamination of aziridines by nitrosyl chloride. *International Journal of Quantum Chemistry*, **2005**, 102, 139-146	2.1	8
92	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
91	Calculation of Franck-Condon factors including anharmonicity: simulation of the C2H4+X2B3u. *Journal of Chemical Physics*, **2005**, 122, 184104	3.9	24
90	The aromatic fluctuation index (FLU): a new aromaticity index based on electron delocalization. *Journal of Chemical Physics*, **2005**, 122, 14109	3.9	321
89	The hardness profile as a tool to detect spurious stationary points in the potential energy surface. *Journal of Chemical Physics*, **2004**, 120, 10914-24	3.9	30
88	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
87	Relation between the substituent effect and aromaticity. *Journal of Organic Chemistry*, **2004**, 69, 6634-40	4.2	163
86	Analysis of electronic delocalization in buckminsterfullerene (C60). *International Journal of Quantum Chemistry*, **2004**, 98, 361-366	2.1	20
85	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, 439-46	3.5	10
84	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
83	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
82	Quantum chemical study of the reactivity of C60HR and C60(CHR) derivatives. *Journal of Organic Chemistry*, **2004**, 69, 2374-80	4.2	8
81	Ground and Low-Lying States of Cu2+H2O. A Difficult Case for Density Functional Methods. *Journal of Physical Chemistry A*, **2004**, 108, 6072-6078	2.8	79
80	Discrepancy between common local aromaticity measures in a series of carbazole derivatives. *Physical Chemistry Chemical Physics*, **2004**, 6, 314-318	3.6	92
79	Stereodiscrimination in Phosphanylthiolato Nickel(II) Complexes. *European Journal of Inorganic Chemistry*, **2003**, 2003, 4147-4151	2.3	14
78	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
77	An insight into the local aromaticities of polycyclic aromatic hydrocarbons and fullerenes. *Chemistry - A European Journal*, **2003**, 9, 1113-22	4.8	113

76	Electron pairing analysis of the Fischer-type chromium□arbene complexes (CO)5Cr?C(X)R (X=H, OH, OCH3, NH2, NHCH3 and R=H, CH3, CH?CH2, Ph, C?CH). *Chemical Physics*, **2003**, 294, 129-139	2.3	17
75	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
74	Evaluation of the Analogy between Exceptions to the Generalized Maximum Hardness Principle for Non-Totally-Symmetric Vibrations and the Pseudo-Jahn□eller Effect. *Journal of Physical Chemistry A*, **2003**, 107, 7337-7339	2.8	15
73	Dinuclear copper(I) complexes with hexaaza macrocyclic dinucleating ligands: structure and dynamic properties. *Inorganic Chemistry*, **2003**, 42, 4456-68	5.1	19
72	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
71	Relations among several nuclear and electronic density functional reactivity indexes. *Journal of Chemical Physics*, **2003**, 119, 9393-9400	3.9	19
70	Electron localization and delocalization in open-shell molecules. *Journal of Computational Chemistry* , **2002**, 23, 1347-56	3.5	31
69	The calculation of electron localization and delocalization indices at the Hartree□ock, density functional and post-Hartree□ock levels of theory. *Theoretical Chemistry Accounts*, **2002**, 107, 362-371	1.9	166
68	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
67	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
66	BIELECTRONIC DENSITIES: ANALYSIS AND APPLICATIONS IN MOLECULAR STRUCTURE AND CHEMICAL REACTIVITY **2002**, 831-870		2
65	Isolation and characterization of four isomers of a C(60) bisadduct with a TTF derivative. Study of their radical ions. *Journal of Organic Chemistry*, **2002**, 67, 566-75	4.2	20
64	Molecular Structure and Bond Characterization of the Fischer-Type Chromium□arbene 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
63	Global Hardness Evaluation Using Simplified Models for the Hardness Kernel. *Journal of Physical Chemistry A*, **2002**, 106, 4632-4638	2.8	27
62	Initial convergence of the perturbation series expansion for vibrational nonlinear optical properties. *Journal of Chemical Physics*, **2002**, 116, 5363-5373	3.9	42
61	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
60	Density functional theory study of the structures and stabilities of CuOdocumentclass{article}pagestyle{empty}begin{document}$_{3}^{-}$end{document} and CuO3. *International Journal of Quantum Chemistry*, **2001**, 81, 162-168	2.1	11
59	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	3.5	15

58	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
57	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
56	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
55	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	3.8	12
54	New Insights in Chemical Reactivity by Means of Electron Pairing Analysis. *Journal of Physical Chemistry A*, **2001**, 105, 2052-2063	2.8	29
53	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	2.8	31
52	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	3.5	10
51	Substituent effects on the intramolecular proton transfer in the ground and lowest-lying singlet excited states of salicylaldimine. *Chemical Physics*, **2000**, 260, 53-64	2.3	20
50	The [2+1] Cycloaddition of Singlet Oxycarbonylnitrenes to C60. *Journal of Molecular Modeling*, **2000**, 6, 205-212	2	14
49	Theoretical Studies of Some Transition-Metal-Mediated Reactions of Industrial and Synthetic Importance. *Chemical Reviews*, **2000**, 100, 439-494	68.1	333
48	Mechanisms for the formation of epoxide and chlorine-containing products in the oxidation of ethylene by chromyl chloride: a density functional study. *Canadian Journal of Chemistry*, **1999**, 77, 1476-1491	0.9	26
47	. *Journal of Physical Chemistry A*, **1999**, 103, 4525-4532	2.8	74
46	Weighing Different Mechanistic Proposals for the DÉz Reaction: A Density Functional Study. *Journal of the American Chemical Society*, **1999**, 121, 1309-1316	16.4	34
45	Excited-State Intramolecular Proton Transfer and Rotamerism of 2-(2Ehydroxyvinyl)benzimidazole and 2-(2Ehydroxyphenyl)imidazole. *Journal of Physical Chemistry A*, **1999**, 103, 4413-4420	2.8	69
44	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
43	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
42	Optimizing hybrid density functionals by means of quantum molecular similarity techniques. *Advances in Molecular Similarity*, **1999**, 187-203		2
41	Exploring the possibility of a bimolecular reaction channel for the F2SS/FSSF rearrangement process. *Computational and Theoretical Chemistry*, **1998**, 455, 123-129		4

40	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	2.1	24
39	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	2.3	21
38	Low-lying electronic states and molecular structure of Fe2O2. *Journal of the Chemical Society, Faraday Transactions*, **1998**, 94, 2877-2881		9
37	Density Functional Study on the Preactivation Scenario of the D□z Reaction: Carbon Monoxide Dissociation versus Alkyne Addition as the First Reaction Step. *Organometallics*, **1998**, 17, 1492-1501	3.8	31
36	Diels-Alder Cycloadditions of 1,3-Butadiene to Polycyclic Aromatic Hydrocarbons (PAH). Quantifying the Reactivity Likeness of Bowl-Shaped PAHs to C(60). *Journal of Organic Chemistry*, **1998**, 63, 7556-7558	4.2	19
35	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
34	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
33	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	3.8	10
32	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	2.7	9
31	Low-lying electronic states and molecular structure of FeO2 and FeO2□ *Chemical Physics Letters*, **1997**, 274, 411-421	2.5	24
30	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
29	Theoretical Study on Acetaldehyde and Ethanol Elimination from the Hydrogenation of CH3(O)CCo(CO)3. *Organometallics*, **1996**, 15, 2611-2618	3.8	48
28	Theoretical Study of the Regioselectivity of Successive 1,3-Butadiene Diels□Alder Cycloadditions to C60. *Journal of the American Chemical Society*, **1996**, 118, 8920-8924	16.4	31
27	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
26	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		25
25	Analysis of the changes on the potential energy surface of Menshutkin reactions induced by external perturbations. *Computational and Theoretical Chemistry*, **1996**, 371, 171-183		25
24	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		22
23	Exploring chromium (VI) dioxodihalides chemistry: Is density functional theory the most suitable tool?. *Journal of Chemical Physics*, **1996**, 104, 9499-9510	3.9	27

22	How similar are HF, MP2, and DFT charge distributions in the Cr(CO)6 complex?. *Advances in Molecular Similarity*, **1996**, 167-186		2
21	The use of ab initio quantum molecular self-similarity measures to analyze electronic charge density distributions **1996**, 58, 361		24
20	Molecular Size and Pyramidalization: Two Keys for Understanding the Reactivity of Fullerenes. *The Journal of Physical Chemistry*, **1995**, 99, 10752-10758		47
19	Ab initio study of the HCO 3 /H2O exchange in the (NH3)3 ZnII(HCO 3) complex. *Theoretica Chimica Acta*, **1995**, 91, 333-351		1
18	AM1 study of a substituent transfer by means of a Diels Alder and retro-Diels Alder tandem reaction. *Journal of the Chemical Society Perkin Transactions II*, **1995**, 605-608		5
17	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
16	Foundations and recent developments on molecular quantum similarity. *Topics in Current Chemistry* , **1995**, 31-62		62
15	An AM1 study of the reactivity of buckminsterfullerene (C60) in a Diels-Alder model reaction. *Chemical Physics Letters*, **1994**, 231, 325-330	2.5	40
14	On the calculation of ab initio quantum molecular similarities for large systems: Fitting the electron density. *Journal of Computational Chemistry*, **1994**, 15, 1113-1120	3.5	44
13	A quantum chemical AM1 study of a Diels Alder and retro-Diels Alder tandem reaction. *Journal of the Chemical Society Perkin Transactions II*, **1994**, 281-284		8
12	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
11	Ab Initio Quantum Molecular Similarity Measures on Metal-Substituted Carbonic Anhydrase (MIICA, M = Be, Mg, Mn, Co, Ni, Cu, Zn, and Cd). *Journal of Chemical Information and Computer Sciences*, **1994**, 34, 1047-1053		22
10	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
9	Valence-bond calculations on ZNO and HGO using integrals computed through the semiempirical AM1 method. *International Journal of Quantum Chemistry*, **1992**, 44, 887-895	2.1	2
8	Ab initio study of the effect of external perturbations in the dissociation of CH3Cl. *Computational and Theoretical Chemistry*, **1992**, 255, 283-296		8
7	Theoretical Study of the Catalyzed Hydration of CO2 by Carbonic Anhydrase: A Brief Overview. **1992**, 263-298		2
6	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	2.1	7
5	Anion binding and pentacoordination in zinc(II) complexes. *Inorganic Chemistry*, **1991**, 30, 2523-2527	5.1	26

4	Analysis of solvent effects on the Menshutkin reaction. *Journal of the American Chemical Society*, **1991**, 113, 2873-2879	16.4	108
3	Ab initio study of substituent effect on the addition of hydrogen fluoride to fluoroethylenes. *Journal of Computational Chemistry*, **1990**, 11, 170-180	3.5	8
2	Aromaticity Analysis by Means of the Quantum Theory of Atoms in Molecules399-423		5
1	One Century of Physical Organic Chemistry: The Menshutkin Reaction. *Progress in Physical Organic Chemistry*,1-182		31