List of Publications by Year in descending order

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| # | Article | IF | CITATIONS |
|----|---|------|-----------|
| 1 | Theoretical Evaluation of Electron Delocalization in Aromatic Molecules by Means of Atoms in Molecules (AIM) and Electron Localization Function (ELF) Topological Approaches. Chemical Reviews, 2005, 105, 3911-3947. | 23.0 | 661 |
| 2 | The Delocalization Index as an Electronic Aromaticity Criterion: Application to a Series of Planar Polycyclic Aromatic Hydrocarbons. Chemistry - A European Journal, 2003, 9, 400-406. | 1.7 | 396 |
| 3 | Quantifying aromaticity with electron delocalisation measures. Chemical Society Reviews, 2015, 44, 6434-6451. | 18.7 | 335 |
| 4 | Hydrogen–Hydrogen Bonding in Planar Biphenyl, Predicted by Atoms-In-Molecules Theory, Does Not Exist. Chemistry - A European Journal, 2006, 12, 2889-2895. | 1.7 | 314 |
| 5 | On the performance of some aromaticity indices: A critical assessment using a test set. Journal of Computational Chemistry, 2008, 29, 1543-1554. | 1.5 | 261 |
| 6 | Ï€â€Aromaticity and Threeâ€Dimensional Aromaticity: Two sides of the Same Coin?. Angewandte Chemie - International Edition, 2014, 53, 12191-12195. | 7.2 | 242 |
| 7 | A Model of the Chemical Bond Must Be Rooted in Quantum Mechanics, Provide Insight, and Possess Predictive Power. Chemistry - A European Journal, 2006, 12, 2902-2905. | 1.7 | 216 |
| 8 | Polycyclic Benzenoids:Â Why Kinked is More Stable than Straight. Journal of Organic Chemistry, 2007, 72, 1134-1142. | 1.7 | 197 |
| 9 | Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1â^'9). Journal of Organic Chemistry, 2005, 70, 2509-2521. | 1.7 | 195 |
| 10 | The calculation of electron localization and delocalization indices at the Hartree-Fock, density functional and post-Hartree-Fock levels of theory. Theoretical Chemistry Accounts, 2002, 107, 362-371. | 0.5 | 187 |
| 11 | Relation between the Substituent Effect and Aromaticity. Journal of Organic Chemistry, 2004, 69, 6634-6640. | 1.7 | 177 |
| 12 | Electron-pairing analysis from localization and delocalization indices in the framework of the atoms-in-molecules theory. Theoretical Chemistry Accounts, 2002, 108, 214-224. | 0.5 | 175 |
| 13 | Comparison of the AIM Delocalization Index and the Mayer and Fuzzy Atom Bond Orders. Journal of Physical Chemistry A, 2005, 109, 9904-9910. | 1.1 | 169 |
| 14 | Assessment of Clar's aromatic π-sextet rule by means of PDI, NICS and HOMA indicators of local aromaticity. Journal of Physical Organic Chemistry, 2005, 18, 785-791. | 0.9 | 147 |
| 15 | Too Persistent to Give Up: Aromaticity in Boron Clusters Survives Radical Structural Changes. Journal of the American Chemical Society, 2020, 142, 9396-9407. | 6.6 | 145 |
| 16 | An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes. Chemistry - A European Journal, 2003, 9, 1113-1122. | 1.7 | 125 |
| 17 | Adenine versus guanine quartets in aqueous solution: dispersion-corrected DFT study on the differences in π-stacking and hydrogen-bonding behavior. Theoretical Chemistry Accounts, 2010, 125, 245-252. | 0.5 | 123 |
| 18 | A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity. Symmetry, 2010, 2, 1156-1179. | 1.1 | 115 |

| # | Article | IF | CITATIONS |
|----|---|-----|-----------|
| 19 | Local Aromaticity of the Six-Membered Rings in Pyracylene. A Difficult Case for the NICS Indicator of Aromaticity. Journal of Organic Chemistry, 2004, 69, 7537-7542. | 1.7 | 113 |
| 20 | <i>para</i> -Selective C–H Olefination of Aniline Derivatives via Pd/S,O-Ligand Catalysis. Journal of the American Chemical Society, 2019, 141, 6719-6725. | 6.6 | 108 |
| 21 | Discrepancy between common local aromaticity measures in a series of carbazole derivatives. Physical Chemistry Chemical Physics, 2004, 6, 314-318. | 1.3 | 106 |
| 22 | Metalloaromaticity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 105-122. | 6.2 | 105 |
| 23 | Hückel's Rule of Aromaticity Categorizes Aromatic <i>closo</i> Boron Hydride Clusters. Chemistry - A European Journal, 2016, 22, 7437-7443. | 1.7 | 103 |
| 24 | Aromaticity of Distorted Benzene Rings:  Exploring the Validity of Different Indicators of Aromaticity. Journal of Physical Chemistry A, 2007, 111, 4513-4521. | 1.1 | 102 |
| 25 | Ground and Low-Lying States of Cu2+â^'H2O. A Difficult Case for Density Functional Methods. Journal of Physical Chemistry A, 2004, 108, 6072-6078. | 1.1 | 85 |
| 26 | A Test to Evaluate the Performance of Aromaticity Descriptors in All-Metal and Semimetal Clusters. An Appraisal of Electronic and Magnetic Indicators of Aromaticity. Journal of Chemical Theory and Computation, 2010, 6, 1118-1130. | 2.3 | 84 |
| 27 | Modeling the structureâ€property relationships of nanoneedles: A journey toward nanomedicine. Journal of Computational Chemistry, 2009, 30, 275-284. | 1.5 | 76 |
| 28 | On the electron-pair nature of the hydrogen bond in the framework of the atoms in molecules theory. Chemical Physics Letters, 2003, 369, 248-255. | 1.2 | 74 |
| 29 | New Solids Based on B ₁₂ N ₁₂ Fullerenes. Journal of Physical Chemistry C, 2007, 111, 13354-13360. | 1.5 | 72 |
| 30 | Chemical basis for the recognition of trimethyllysine by epigenetic reader proteins. Nature Communications, 2015, 6, 8911. | 5.8 | 72 |
| 31 | A trinuclear Pt(ii) compound with short Pt–Pt–Pt contacts. An analysis of the influence of π–π stacking interactions on the strength and length of the Pt–Pt bond. Dalton Transactions, 2006, , 1188-1196. | 1.6 | 70 |
| 32 | Local Aromaticity of the Lowest-Lying Singlet States of [n]Acenes (n = 6â^'9). Journal of Physical Chemistry A, 2005, 109, 10629-10632. | 1.1 | 68 |
| 33 | Double CH Activation of a Masked Cationic Bismuth Amide. Angewandte Chemie - International Edition, 2018, 57, 3825-3829. | 7.2 | 66 |
| 34 | B-DNA structure and stability: the role of hydrogen bonding, π–π stacking interactions, twist-angle, and solvation. Organic and Biomolecular Chemistry, 2014, 12, 4691-4700. | 1.5 | 64 |
| 35 | 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. | 1.5 | 59 |
| 36 | Carbon monoxide insertion at a heavy p-block element: unprecedented formation of a cationic bismuth carbamoyl. Chemical Science, 2019, 10, 4169-4176. | 3.7 | 59 |

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| 37 | Role of Electron Density and Magnetic Couplings on the Nucleus-Independent Chemical Shift (NICS) Profiles of [2.2]Paracyclophane and Related Species. Journal of Organic Chemistry, 2006, 71, 1700-1702. | 1.7 | 57 |
| 38 | Aromaticity and electronic delocalization in all-metal clusters with single, double, and triple aromatic character. Theoretical Chemistry Accounts, 2011, 128, 419-431. | 0.5 | 57 |
| 39 | PyFrag 2019—Automating the exploration and analysis of reaction mechanisms. Journal of Computational Chemistry, 2019, 40, 2227-2233. | 1.5 | 57 |
| 40 | Covalent and Ionic Capacity of MOFs To Sorb Small Gas Molecules. Inorganic Chemistry, 2018, 57, 6981-6990. | 1.9 | 55 |
| 41 | Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. Journal of Physical Chemistry A, 2006, 110, 12249-12258. | 1.1 | 52 |
| 42 | Selectivity in DNA replication. Interplay of steric shape, hydrogen bonds, π-stacking and solvent effects. Chemical Communications, 2011, 47, 7326. | 2.2 | 52 |
| 43 | Analysis of the effect of changing the a0 parameter of the Becke3-LYP hybrid functional on the transition state geometries and energy barriers in a series of prototypical reactions. Physical Chemistry Chemical Physics, 2002, 4, 722-731. | 1.3 | 51 |
| 44 | Open-shell spherical aromaticity: the 2N2 + 2N + 1 (with S = N + $\hat{A}^{1/2}$) rule. Chemical Communications, 2011, 47, 11647. | 2.2 | 49 |
| 45 | Reactivity of the Donorâ€6tabilized Silylenes [<i>i</i> PrNC(Ph)N <i>i</i> Pr] ₂ Si and [<i>i</i> PrNC(N <i>i</i> Pr ₂)N <i>i</i> Pr] ₂ Si: Activation of CO ₂ and CS ₂ . Chemistry - A European Journal, 2015, 21, 16665-16672. | 1.7 | 49 |
| 46 | Nuclear magnetic resonance chemical shifts with the statistical average of orbital-dependent model potentials in Kohn–Sham density functional theory. Journal of Chemical Physics, 2003, 118, 8584-8593. | 1.2 | 48 |
| 47 | Aromaticity Analysis of Lithium Cation/ π Complexes of Aromatic Systems. ChemPhysChem, 2005, 6, 2552-2561. | 1.0 | 46 |
| 48 | Analysis of the Effects ofN-Substituents on Some Aspects of the Aromaticity of Imidazoles and Pyrazoles. Journal of Physical Chemistry A, 2011, 115, 8571-8577. | 1.1 | 46 |
| 49 | The Missing Entry in the Agostic–Anagostic Series: Rh(I)–η ¹ -C Interactions in P(CH)P Pincer Complexes. Inorganic Chemistry, 2015, 54, 2960-2969. | 1.9 | 46 |
| 50 | Electron Fluctuation in Pericyclic and Pseudopericyclic Reactions. ChemPhysChem, 2006, 7, 111-113. | 1.0 | 45 |
| 51 | An Analysis of the Isomerization Energies of 1,2-/1,3-Diazacyclobutadiene, Pyrazole/Imidazole, and Pyridazine/Pyrimidine with the Turn-Upside-Down Approach. Journal of Organic Chemistry, 2011, 76, 8913-8921. | 1.7 | 43 |
| 52 | Aromaticity Determines the Relative Stability of Kinked vs. Straight Topologies in Polycyclic Aromatic Hydrocarbons. Frontiers in Chemistry, 2018, 6, 561. | 1.8 | 41 |
| 53 | A Simple Link between Hydrocarbon and Borohydride Chemistries. Chemistry - A European Journal, 2013, 19, 4169-4175. | 1.7 | 40 |
| 54 | Bonding in Methylalkalimetals (CH3M)n(M = Li, Na, K;n= 1, 4). Agreement and Divergences between AIM and ELF Analysesâ€. Journal of Physical Chemistry B, 2006, 110, 7189-7198. | 1.2 | 39 |

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| 55 | Didehydrophenanthrenes:  Structure, Singletâ^'Triplet Splitting, and Aromaticity. Journal of Physical Chemistry A, 2007, 111, 5063-5070. | 1.1 | 39 |
| 56 | Analysis of Hückel's [4 <i>n</i> + 2] Rule through Electronic Delocalization Measures. Journal of Physical Chemistry A, 2008, 112, 13231-13238. | 1.1 | 38 |
| 57 | Patterns of ï€-electron delocalization in aromatic and antiaromatic organic compounds in the light of Hückel's 4n + 2 rule. Physical Chemistry Chemical Physics, 2010, 12, 7126. | 1.3 | 38 |
| 58 | Examining the Planarity of Poly(3,4-ethylenedioxythiophene): Consideration of Self-Rigidification, Electronic, and Geometric Effects. Journal of Physical Chemistry A, 2010, 114, 1023-1028. | 1.1 | 38 |
| 59 | Hypervalent versus Nonhypervalent Carbon in Nobleâ€Gas Complexes. Chemistry - A European Journal, 2008, 14, 6901-6911. | 1.7 | 37 |
| 60 | Analysis of the Relative Stabilities of Ortho, Meta, and Para MClY(XC ₄ H ₄)(PH ₃) ₂ Heterometallabenzenes (M = Rh,) Tj ET | Q±q£0 00r | g Bi 6/Overloo |
| 61 | Bismuth Amides Mediate Facile and Highly Selective Pn–Pn Radicalâ€Coupling Reactions (Pn=N, P, As). Angewandte Chemie - International Edition, 2021, 60, 6441-6445. | 7.2 | 36 |
| 62 | New Insights in Chemical Reactivity by Means of Electron Pairing Analysis. Journal of Physical Chemistry A, 2001, 105, 2052-2063. | 1.1 | 34 |
| 63 | Are nucleus-independent (NICS) and 1H NMR chemical shifts good indicators of aromaticity in ï€-stacked polyfluorenes?. Chemical Physics Letters, 2006, 428, 191-195. | 1.2 | 33 |
| 64 | Effects of Solvation on the Pairing of Electrons in a Series of Simple Molecules and in the Menshutkin Reaction. Journal of Physical Chemistry A, 2001, 105, 6249-6257. | 1.1 | 32 |
| 65 | Hydrogen bonding and aromaticity in the guanine–cytosine base pair interacting with metal cations (M = Cu+, Ca2+and Cu2+). Molecular Physics, 2005, 103, 163-173. | 0.8 | 32 |
| 66 | Solvent effects on hydrogen bonds in Watson–Crick, mismatched, and modified DNA base pairs. Computational and Theoretical Chemistry, 2012, 998, 57-63. | 1.1 | 32 |
| 67 | The <i>nido</i> ageâ<â<ï€ Bond: A Nonâ€covalent Interaction between Boron Clusters and Aromatic Ri and Its Applications. Angewandte Chemie - International Edition, 2020, 59, 9018-9025. | ngs 7.2 | 32 |
| 68 | Analysis of the Aromaticity of Five-Membered Heterometallacycles Containing Os, Ru, Rh, and Ir. Organometallics, 2014, 33, 1762-1773. | 1.1 | 31 |
| 69 | Understanding Conjugation and Hyperconjugation from Electronic Delocalization Measures. Journal of Physical Chemistry A, 2011, 115, 13104-13113. | 1.1 | 30 |
| 70 | Stable Fourâ€Coordinate Guanidinatosilicon(IV) Complexes with SiN 3 El Skeletons (El=S, Se, Te) and SiEl Double Bonds. Chemistry - A European Journal, 2015, 21, 14011-14021. | 1.7 | 29 |
| 71 | Analysis of Electron Delocalization in Aromatic Systems:  Individual Molecular Orbital Contributions to Para-Delocalization Indexes (PDI). Journal of Physical Chemistry A, 2006, 110, 11569-11574. | 1.1 | 28 |
| 72 | Path-dependency of energy decomposition analysis & the elusive nature of bonding. Physical Chemistry Chemical Physics, 2022, 24, 2344-2348. | 1.3 | 27 |

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| 73 | Rational design of nearâ€infrared absorbing organic dyes: Controlling the HOMO–LUMO gap using quantitative molecular orbital theory. Journal of Computational Chemistry, 2018, 39, 2690-2696. | 1.5 | 26 |
| 74 | The Chemical Bond: When Atom Size Instead of Electronegativity Difference Determines Trend in Bond Strength. Chemistry - A European Journal, 2021, 27, 15616-15622. | 1.7 | 26 |
| 75 | B-DNA model systems in non-terran bio-solvents: implications for structure, stability and replication. Physical Chemistry Chemical Physics, 2017, 19, 16969-16978. | 1.3 | 25 |
| 76 | Doppelte CHâ€Aktivierung eines maskierten Bismutamidâ€Kations. Angewandte Chemie, 2018, 130, 3887-3891. | 1.6 | 25 |
| 77 | Exploring the validity of the Glidewell–Lloyd extension of Clar's π-sextet rule: assessment from polycyclic conjugated hydrocarbons. Theoretical Chemistry Accounts, 2016, 135, 1. | 0.5 | 24 |
| 78 | Analysis of electronic delocalization in buckminsterfullerene (C60). International Journal of Quantum Chemistry, 2004, 98, 361-366. | 1.0 | 23 |
| 79 | Reaction Mechanism and Regioselectivity of the Bingel–Hirsch Addition of Dimethyl Bromomalonate to La@ <i>C</i> _{2<i>v</i>} ₈₂ . Chemistry - A European Journal, 2016, 22, 5953-5962. | 1.7 | 23 |
| 80 | 3D and 2D aromatic units behave like oil and water in the case of benzocarborane derivatives. Nature Communications, 2022, 13, . | 5.8 | 23 |
| 81 | Diastereoselective Synthesis of Fulleropyrrolidines from Suitably Functionalized Chiral Cyclobutanes. Journal of Organic Chemistry, 2005, 70, 6929-6932. | 1.7 | 22 |
| 82 | Parametrization of the Becke3-LYP hybrid functional for a series of small molecules using quantum molecular similarity techniques. Journal of Computational Chemistry, 2001, 22, 1666-1678. | 1.5 | 21 |
| 83 | On the electronic structure of second generation Hoveyda–Grubbs alkene metathesis precursors. Computational and Theoretical Chemistry, 2012, 996, 57-67. | 1.1 | 21 |
| 84 | Ab Initio Design of Chelating Ligands Relevant to Alzheimer's Disease: Influence of Metalloaromaticity. Journal of Physical Chemistry A, 2011, 115, 12659-12666. | 1.1 | 20 |
| 85 | Electron pairing analysis of the Fischer-type chromium–carbene complexes (CO)5CrĩC(X)R (X=H, OH,) Tj ETQ | q110.784 | 4314 rgBT 18 |
| 86 | Aromaticity changes along the reaction coordinate connecting the cyclobutadiene dimer to cubane and the benzene dimer to hexaprismane. Structural Chemistry, 2007, 18, 773-783. | 1.0 | 18 |
| 87 | Molecular structures of M2N22â^' (M and N = B, Al, and Ga) clusters using the gradient embedded genetic algorithm. Physical Chemistry Chemical Physics, 2012, 14, 14850. | 1.3 | 18 |
| 88 | Stabilization of 2,6-Diarylanilinum Cation by Through-Space Cationâ^'Ï€ Interactions. Journal of Organic Chemistry, 2017, 82, 9418-9424. | 1.7 | 18 |
| 89 | 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, 7591-7593. | 1.2 | 17 |
| 90 | Fmoc–RGDS based fibrils: atomistic details of their hierarchical assembly. Physical Chemistry Chemical Physics, 2016, 18, 1265-1278. | 1.3 | 17 |

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| 91 | Kekulene: Structure, stability and nature of H•••H interactions in large PAHs. Molecular Astrophysics, 2017, 8, 19-26. | 1.7 | 17 |
| 92 | Theoretical studies on aromaticity of selected hydroxypyrones. Part 3#. Chelatoaromaticity phenomenon in metalcomplexes of hydroxypyrones. Journal of Physical Organic Chemistry, 2011, 24, 499-506. | 0.9 | 16 |
| 93 | X ₂ Y ₂ lsomers: Tuning Structure and Relative Stability through Electronegativity Differences (X = H, Li, Na, F, Cl, Br, I; Y = O, S, Se, Te). Inorganic Chemistry, 2013, 52, 2458-2465. | 1.9 | 16 |
| 94 | Why 1,2-quinone derivatives are more stable than their 2,3-analogues?. Theoretical Chemistry Accounts, 2015, 134, 1. | 0.5 | 16 |
| 95 | Alkali Metal Complexes of Silyl-Substitutedansa-(Tris)allyl Ligands: Metal-, Co-Ligand- and Substituent-Dependent Stereochemistry. European Journal of Inorganic Chemistry, 2009, 2009, 4157-4167. | 1.0 | 15 |
| 96 | Routes of π-Electron Delocalization in 4-Substituted-1,2-benzoquinones. Journal of Organic Chemistry, 2011, 76, 550-556. | 1.7 | 15 |
| 97 | Recognition of shorter and longer trimethyllysine analogues by epigenetic reader proteins. Chemical Communications, 2018, 54, 2409-2412. | 2.2 | 15 |
| 98 | Open-shell jellium aromaticity in metal clusters. Chemical Communications, 2019, 55, 5559-5562. | 2.2 | 15 |
| 99 | A donor-functionalized, silyl-substituted pentadienyllithium: structural insight from experiment and theory. Chemical Communications, 2011, 47, 6162. | 2.2 | 14 |
| 100 | All-metal aromatic clusters M42â^' (M = B, Al, and Ga). Are Ï€-electrons distortive or not?. Physical Chemistry Chemical Physics, 2011, 13, 20673. | 1.3 | 14 |
| 101 | Formation of a Trifluorophosphane Platinum(II) Complex by Pâ^'F Bond Activation of Phosphorus Pentafluoride with a Pt ⁰ Complex. Chemistry - A European Journal, 2017, 23, 5948-5952. | 1.7 | 14 |
| 102 | Binding of 6-mer single-stranded homo-nucleotides to poly(3,4-ethylenedioxythiophene): specific hydrogen bonds with guanine. Soft Matter, 2011, 7, 9922. | 1.2 | 13 |
| 103 | Unraveling the Origin of the Relative Stabilities of Group 14 M ₂ N ₂ ²⁺ (M, N = C, Si, Ge, Sn, and Pb) Isomer Clusters. Journal of Physical Chemistry A, 2013, 117, 10462-10469. | 1.1 | 13 |
| 104 | Mechanism of biomolecular recognition of trimethyllysine by the fluorinated aromatic cage of KDM5A PHD3 finger. Communications Chemistry, 2020, 3, . | 2.0 | 13 |
| 105 | Octahedral aromaticity in ^{2S+1} A _{1g} X ₆ ^q clusters (X =) Tj ET | Qq110.7 | 784314 rgBT |
| 106 | Understanding the differences between iron and palladium in cross-coupling reactions. Physical Chemistry Chemical Physics, 2019, 21, 9651-9664. | 1.3 | 12 |
| 107 | Distortionâ€Controlled Redshift of Organic Dye Molecules. Chemistry - A European Journal, 2020, 26, 2080-2093. | 1.7 | 12 |
| 108 | Analysis of the electronic delocalization in some isoelectronic analogues of B ₁₂ doped with beryllium and/or carbon. Physical Chemistry Chemical Physics, 2020, 22, 12245-12259. | 1.3 | 12 |

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| 109 | Aromaticity and Extrusion of Benzenoids Linked to [<i>o</i> OSAN] ^{â^'} : Clar Has the Answer. Angewandte Chemie - International Edition, 2022, 61, . | 7.2 | 12 |
| 110 | Nature of the Ruâ^'NO Coordination Bond: Kohn–Sham Molecular Orbital and Energy Decomposition Analysis. ChemistryOpen, 2017, 6, 410-416. | 0.9 | 11 |
| 111 | Probing Through-Space Polarâ^ï€ Interactions in 2,6-Diarylphenols. Journal of Organic Chemistry, 2019, 84, 3632-3637. | 1.7 | 11 |
| 112 | Probing Halogenâ~'Ï€ versus CHâ^'Ï€ Interactions in Molecular Balance. Organic Letters, 2020, 22, 7870-7873. | 2.4 | 11 |
| 113 | Câ^'X Bond Activation by Palladium: Steric Shielding versus Steric Attraction. Chemistry - A European Journal, 2022, 28, . | 1.7 | 11 |
| 114 | Complexes of adamantaneâ€based group 13 Lewis acids and superacids: Bonding analysis and thermodynamics of hydrogen splitting. Journal of Computational Chemistry, 2016, 37, 1355-1362. | 1.5 | 10 |
| 115 | Ab initio and DFT modeling of stereoselective deamination of aziridines by nitrosyl chloride. International Journal of Quantum Chemistry, 2005, 102, 139-146. | 1.0 | 9 |
| 116 | Excess charge delocalization in organic and biological molecules: some theoretical notions. Theoretical Chemistry Accounts, 2009, 123, 29-40. | 0.5 | 9 |
| 117 | Comparison between Alkalimetal and Group 11 Transition Metal Halide and Hydride Tetramers: Molecular Structure and Bonding. Journal of Physical Chemistry A, 2013, 117, 8026-8034. | 1.1 | 9 |
| 118 | Aromaticity and Magnetic Properties of 1―and 2â€Indenones and Their Aza Derivatives. European Journal of Organic Chemistry, 2014, 2014, 5370-5377. | 1.2 | 9 |
| 119 | Testing the effectiveness of the isoelectronic substitution principle through the transformation of aromatic osmathiophene derivatives into their inorganic analogues. New Journal of Chemistry, 2017, 41, 1168-1178. | 1.4 | 9 |
| 120 | Through‧pace Polarâ€ï€ Interactions in 2,6â€Diarylthiophenols. ChemPhysChem, 2020, 21, 1092-1100. | 1.0 | 9 |
| 121 | Properties of poly(3-halidethiophene)s. Physical Chemistry Chemical Physics, 2012, 14, 10050. | 1.3 | 8 |
| 122 | Aromatic properties of 8-hydroxyquinoline and its metal complexes. Open Chemistry, 2013, 11, 655-663. | 1.0 | 8 |
| 123 | Comparison of Molecular Recognition of Trimethyllysine and Trimethylthialysine by Epigenetic Reader Proteins. Molecules, 2020, 25, 1918. | 1.7 | 8 |
| 124 | The energy components of the extended transition state energy decomposition analysis are path functions: the case of water tetramer. Theoretical Chemistry Accounts, 2021, 140, 1. | 0.5 | 8 |
| 125 | Probing the Lewis Acidity of Boronic Acids through Interactions with Arene Substituents. Chemistry - A European Journal, 2022, 28, . | 1.7 | 8 |
| 126 | Examining the formation of specific interactions between poly(3,4-ethylenedioxythiophene) and nucleotide bases. RSC Advances, 2013, 3, 2639. | 1.7 | 7 |

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| 127 | Rules of Aromaticity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 321-335. | 0.6 | 7 |
| 128 | Planar <i>vs.</i> three-dimensional X ₆ ^{2â^'} , X ₂ Y ₄ ^{2â^'} , and X ₃ Y ₃ ^{2â^'} (X, Y = B,) | Tj ETQq0 | 0.0 rgBT /0\ |
| 129 | Physical Chemistry Chemical Physics, 2016, 18, 21102-21110. Silyleneâ€Induced Reduction of [Mn ₂ (CO) ₁₀]: Formation of a Fiveâ€Coordinate Silicon(IV) Complex with an Oâ€Bound [(OC) ₄ Mn=Mn(CO) ₄] ^{2â€"} Ligand. European Journal of Inorganic Chemistry, 2017, 2017, 186-191. | 1.0 | 7 |
| 130 | Phenoxylation of Alkynes through Mono―and Dual Activation Using Group 11 (Cu, Ag, Au) Catalysts. European Journal of Inorganic Chemistry, 2020, 2020, 1123-1134. | 1.0 | 7 |
| 131 | The nido ageâ‹â‹â‹ï€ Bond: A Non ovalent Interaction between Boron Clusters and Aromatic Rings an Applications. Angewandte Chemie, 2020, 132, 9103-9110. | d Its 1.6 | 7 |
| 132 | Bismutamide als einfache Vermittler hochselektiver Pnâ^'Pnâ€Radikalâ€Kupplungsreaktionen (Pn=N, P, As). Angewandte Chemie, 2021, 133, 6513-6518. | 1.6 | 7 |
| 133 | Do Sulfonamides Interact with Aromatic Rings?. Chemistry - A European Journal, 2021, 27, 5721-5729. | 1.7 | 7 |
| 134 | C(<i>sp</i> ⁿ)â^'X (n=1–3) Bond Activation by Palladium. Chemistry - A European Journal, 2022, 28, . | 1.7 | 7 |
| 135 | Rational design of iron catalysts for C – X bond activation. Journal of Computational Chemistry, 2022, , . | 1.5 | 7 |
| 136 | Aromaticity Analysis by Means of the Quantum Theory of Atoms in Molecules. , 0, , 399-423. | | 6 |
| 137 | Electroactive polymers for the detection of morphine. Journal of Polymer Research, 2014, 21, 1. | 1.2 | 6 |
| 138 | How carbo-benzenes fit molecules in their inner core as do biologic ion carriers?. Structural Chemistry, 2016, 27, 249-259. | 1.0 | 6 |
| 139 | Chelation enforcing a dual gold configuration in the catalytic hydroxyphenoxylation of alkynes. Applied Organometallic Chemistry, 2021, 35, e6362. | 1.7 | 5 |
| 140 | Cage [–] ···Cage [–] Interaction: Boron Cluster-Based Noncovalent Bond and Its Applications in Solid-State Materials. Jacs Au, 2021, 1, 2047-2057. | 3.6 | 5 |
| 141 | Aromaticity and Chemical Reactivity. , 2009, , . | | 5 |
| 142 | Zwitterionic Aromaticity on Azulene Extrapolated to <i>carbo</i> â€Azulene. European Journal of Organic Chemistry, 2021, 2021, 6450-6458. | 1.2 | 5 |
| 143 | Reading and erasing of the phosphonium analogue of trimethyllysine by epigenetic proteins. Communications Chemistry, 2022, 5, . | 2.0 | 5 |
| 144 | Activation Strain Analyses of Counterion and Solvent Effects on the Ionâ€Pair S N 2 Reaction of and CH 3 Cl. Journal of Computational Chemistry, 2020, 41, 317-327. | 1.5 | 4 |

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| 145 | Pyrrole and Pyridine in the Water Environment—Effect of Discrete and Continuum Solvation Models. ACS Omega, 2021, 6, 24693-24699. | 1.6 | 4 |
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