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<br>Molecules (AIM) and Electron Localization Function (ELF) Topological Approaches. Chemical Reviews,<br>2005, 105, 3911-3947. | 23.0 | 661       |
| 2  | The Delocalization Index as an Electronic Aromaticity Criterion: Application to a Series of Planar<br>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<br>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<br>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 -<br>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<br>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,<br>72, 1134-1142.                                                                                                      | 1.7  | 197       |
| 9  | Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1â^'9). Journal of Organic<br>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<br>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.<br>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.<br>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<br>differences in π-stacking and hydrogen-bonding behavior. Theoretical Chemistry Accounts, 2010, 125,<br>245-252.               | 0.5  | 123       |
| 18 | A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity.<br>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<br>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<br>European Journal, 2016, 22, 7437-7443.                                                                                                          | 1.7 | 103       |
| 24 | Aromaticity of Distorted Benzene Rings:  Exploring the Validity of Different Indicators of Aromaticity.<br>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<br>Appraisal of Electronic and Magnetic Indicators of Aromaticity. Journal of Chemical Theory and<br>Computation, 2010, 6, 1118-1130.             | 2.3 | 84        |
| 27 | Modeling the structureâ€property relationships of nanoneedles: A journey toward nanomedicine.<br>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 <sub>12</sub> N <sub>12</sub> 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<br>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<br>stacking interactions on the strength and length of the Pt–Pt bond. Dalton Transactions, 2006, ,<br>1188-1196.                                        | 1.6 | 70        |
| 32 | Local Aromaticity of the Lowest-Lying Singlet States of [n]Acenes (n = 6â^'9). Journal of Physical<br>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,<br>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<br>Diels–Alder reaction. Exploring the validity of different indicators of aromaticity. Computational and<br>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        |

| #  | Article                                                                                                                                                                                                                                                                                          | IF  | CITATIONS |
|----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|-----------|
| 37 | Role of Electron Density and Magnetic Couplings on the Nucleus-Independent Chemical Shift (NICS)<br>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<br>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,<br>6981-6990.                                                                                                                                                                                    | 1.9 | 55        |
| 41 | Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. Journal of<br>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<br>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] <sub>2</sub> Si and<br>[ <i>i</i> PrNC(N <i>i</i> Pr <sub>2</sub> )N <i>i</i> Pr] <sub>2</sub> Si: Activation of CO <sub>2</sub> and<br>CS <sub>2</sub> . 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 <sup>1</sup> -C Interactions in P(CH)P Pincer<br>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<br>Pyridazine/Pyrimidine with the Turn-Upside-Down Approach. Journal of Organic Chemistry, 2011, 76,<br>8913-8921.                                                                            | 1.7 | 43        |
| 52 | Aromaticity Determines the Relative Stability of Kinked vs. Straight Topologies in Polycyclic Aromatic<br>Hydrocarbons. Frontiers in Chemistry, 2018, 6, 561.                                                                                                                                    | 1.8 | 41        |
| 53 | A Simple Link between Hydrocarbon and Borohydride Chemistries. Chemistry - A European Journal, 2013,<br>19, 4169-4175.                                                                                                                                                                           | 1.7 | 40        |
| 54 | Bonding in Methylalkalimetals (CH3M)n(M = Li, Na, K;n= 1, 4). Agreement and Divergences between AIM<br>and ELF Analysesâ€. Journal of Physical Chemistry B, 2006, 110, 7189-7198.                                                                                                                | 1.2 | 39        |

| #  | Article                                                                                                                                                                                                | IF               | CITATIONS             |
|----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|-----------------------|
| 55 | Didehydrophenanthrenes:  Structure, Singletâ^'Triplet Splitting, and Aromaticity. Journal of Physical<br>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<br>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<br>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,<br>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,<br>2008, 14, 6901-6911.                                                                              | 1.7              | 37                    |
| 60 | Analysis of the Relative Stabilities of Ortho, Meta, and Para<br>MClY(XC <sub>4</sub> H <sub>4</sub> )(PH <sub>3</sub> ) <sub>2</sub> Heterometallabenzenes (M = Rh,) Tj ET                            | <b>Q±q£0</b> 00r | g <b>Bi</b> 6/Overloo |
| 61 | Bismuth Amides Mediate Facile and Highly Selective Pn–Pn Radicalâ€Coupling Reactions (Pn=N, P, As).<br>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<br>Chemistry A, 2001, 105, 2052-2063.                                                                   | 1.1              | 34                    |
| 63 | Are nucleus-independent (NICS) and 1H NMR chemical shifts good indicators of aromaticity in<br>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<br>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<br>(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.<br>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<br>and Its Applications. Angewandte Chemie - International Edition, 2020, 59, 9018-9025.            | ngs<br>7.2       | 32                    |
| 68 | Analysis of the Aromaticity of Five-Membered Heterometallacycles Containing Os, Ru, Rh, and Ir.<br>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<br>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<br>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<br>Chemistry Chemical Physics, 2022, 24, 2344-2348.                                                         | 1.3              | 27                    |

| #  | Article                                                                                                                                                                                                         | IF       | CITATIONS       |
|----|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-----------------|
| 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<br>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.<br>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<br>Quantum Chemistry, 2004, 98, 361-366.                                                                          | 1.0      | 23              |
| 79 | Reaction Mechanism and Regioselectivity of the Bingel–Hirsch Addition of Dimethyl Bromomalonate<br>to La@ <i>C</i> <sub>2<i>v</i></sub> <sub>82</sub> . Chemistry - A European Journal, 2016, 22,<br>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<br>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.<br>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.<br>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<br>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<br>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<br>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<br>Chemical Physics, 2016, 18, 1265-1278.                                                                         | 1.3      | 17              |

| #   | Article                                                                                                                                                                                                                  | IF      | CITATIONS   |
|-----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------------|
| 91  | Kekulene: Structure, stability and nature of H•••H interactions in large PAHs. Molecular Astrophysics,<br>2017, 8, 19-26.                                                                                                | 1.7     | 17          |
| 92  | Theoretical studies on aromaticity of selected hydroxypyrones. Part 3#. Chelatoaromaticity<br>phenomenon in metalcomplexes of hydroxypyrones. Journal of Physical Organic Chemistry, 2011, 24,<br>499-506.               | 0.9     | 16          |
| 93  | X <sub>2</sub> Y <sub>2</sub> lsomers: Tuning Structure and Relative Stability through<br>Electronegativity Differences (X = H, Li, Na, F, Cl, Br, I; Y = O, S, Se, Te). Inorganic Chemistry, 2013, 52,<br>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<br>Substituent-Dependent Stereochemistry. European Journal of Inorganic Chemistry, 2009, 2009,<br>4157-4167.                 | 1.0     | 15          |
| 96  | Routes of π-Electron Delocalization in 4-Substituted-1,2-benzoquinones. Journal of Organic<br>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<br>Chemistry Chemical Physics, 2011, 13, 20673.                                                                    | 1.3     | 14          |
| 101 | Formation of a Trifluorophosphane Platinum(II) Complex by Pâ^'F Bond Activation of Phosphorus<br>Pentafluoride with a Pt <sup>0</sup> 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<br>M <sub>2</sub> N <sub>2</sub> <sup>2+</sup> (M, N = C, Si, Ge, Sn, and Pb) Isomer Clusters. Journal of<br>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 <sup>2S+1</sup> A <sub>1g</sub> X <sub>6</sub> <sup>q</sup> clusters (X =) Tj ET                                                                                                               | Qq110.7 | 784314 rgBT |
| 106 | Understanding the differences between iron and palladium in cross-coupling reactions. Physical<br>Chemistry Chemical Physics, 2019, 21, 9651-9664.                                                                       | 1.3     | 12          |
| 107 | Distortionâ€Controlled Redshift of Organic Dye Molecules. Chemistry - A European Journal, 2020, 26,<br>2080-2093.                                                                                                        | 1.7     | 12          |
| 108 | Analysis of the electronic delocalization in some isoelectronic analogues of B <sub>12</sub> doped with beryllium and/or carbon. Physical Chemistry Chemical Physics, 2020, 22, 12245-12259.                             | 1.3     | 12          |

| #   | Article                                                                                                                                                                                                                     | IF  | CITATIONS |
|-----|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|-----------|
| 109 | Aromaticity and Extrusion of Benzenoids Linked to [ <i>o</i> OSAN] <sup>â^'</sup> : Clar Has the<br>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<br>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,<br>84, 3632-3637.                                                                                                    | 1.7 | 11        |
| 112 | Probing Halogenâ~'Ï€ versus CHâ^'Ï€ Interactions in Molecular Balance. Organic Letters, 2020, 22,<br>7870-7873.                                                                                                             | 2.4 | 11        |
| 113 | Câ^'X Bond Activation by Palladium: Steric Shielding versus Steric Attraction. Chemistry - A European<br>Journal, 2022, 28, .                                                                                               | 1.7 | 11        |
| 114 | Complexes of adamantaneâ€based group 13 Lewis acids and superacids: Bonding analysis and<br>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.<br>International Journal of Quantum Chemistry, 2005, 102, 139-146.                                                            | 1.0 | 9         |
| 116 | Excess charge delocalization in organic and biological molecules: some theoretical notions.<br>Theoretical Chemistry Accounts, 2009, 123, 29-40.                                                                            | 0.5 | 9         |
| 117 | Comparison between Alkalimetal and Group 11 Transition Metal Halide and Hydride Tetramers:<br>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<br>aromatic osmathiophene derivatives into their inorganic analogues. New Journal of Chemistry, 2017,<br>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<br>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 -<br>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         |

| #   | Article                                                                                                                                                                                                                                                                                                                                           | IF           | CITATIONS    |
|-----|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|--------------|
| 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 <sub>6</sub> <sup>2â^'</sup> ,<br>X <sub>2</sub> Y <sub>4</sub> <sup>2â^'</sup> , and X <sub>3</sub> Y <sub>3</sub> <sup>2â^'</sup> (X, Y = B,)                                                                                                                                                             | Tj ETQq0     | 0.0 rgBT /0\ |
| 129 | Physical Chemistry Chemical Physics, 2016, 18, 21102-21110.<br>Silyleneâ€Induced Reduction of [Mn <sub>2</sub> (CO) <sub>10</sub> ]: Formation of a Fiveâ€Coordinate<br>Silicon(IV) Complex with an Oâ€Bound [(OC) <sub>4</sub> Mn=Mn(CO) <sub>4</sub> ] <sup>2â€"</sup><br>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.<br>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<br>Applications. Angewandte Chemie, 2020, 132, 9103-9110.                                                                                                                                                                                      | d Its<br>1.6 | 7            |
| 132 | Bismutamide als einfache Vermittler hochselektiver Pnâ^'Pnâ€Radikalâ€Kupplungsreaktionen (Pn=N, P, As).<br>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> <sup>n</sup> )â^'X (n=1–3) Bond Activation by Palladium. Chemistry - A European Journal,<br>2022, 28, .                                                                                                                                                                                                                              | 1.7          | 7            |
| 135 | Rational design of iron catalysts for C – X bond activation. Journal of Computational Chemistry, 2022,<br>, .                                                                                                                                                                                                                                     | 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.<br>Applied Organometallic Chemistry, 2021, 35, e6362.                                                                                                                                                                                             | 1.7          | 5            |
| 140 | Cage <sup>–</sup> ···Cage <sup>–</sup> Interaction: Boron Cluster-Based Noncovalent Bond and Its<br>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<br>Organic Chemistry, 2021, 2021, 6450-6458.                                                                                                                                                                                                      | 1.2          | 5            |
| 143 | Reading and erasing of the phosphonium analogue of trimethyllysine by epigenetic proteins.<br>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<br>3 Cl. Journal of Computational Chemistry, 2020, 41, 317-327.                                                                                                                                                                            | 1.5          | 4            |

| #   | Article                                                                                                                                                                                                                                          | IF  | CITATIONS |
|-----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|-----------|
| 145 | Pyrrole and Pyridine in the Water Environment—Effect of Discrete and Continuum Solvation Models.<br>ACS Omega, 2021, 6, 24693-24699.                                                                                                             | 1.6 | 4         |
| 146 | Synthesis and Hydrolysis of Alkoxy(aminoalkyl)diorganylsilanes of the Formula Type<br>R2(RO)Si(CH2)nNH2(R = Alkyl,n= 1-3): A Systematic Experimental and Computational Study. European<br>Journal of Inorganic Chemistry, 2016, 2016, 1641-1659. | 1.0 | 3         |
| 147 | Aromaticity and Extrusion of Benzenoids Linked to [ <i>o</i> â€COSAN] <sup>â^'</sup> : Clar Has the<br>Answer. Angewandte Chemie, 0, , .                                                                                                         | 1.6 | 3         |
| 148 | Cyclopropenylidenephosphoranes: Rearrangement to Azetidinylidene-Methylphosphoniums. Journal of<br>Organic Chemistry, 2020, 85, 7452-7458.                                                                                                       | 1.7 | 2         |
| 149 | Probing Noncovalent Interactions in [3,3]Metaparacyclophanes. Journal of Organic Chemistry, 2022, 87, 6087-6096.                                                                                                                                 | 1.7 | 2         |
| 150 | Through-Space Stabilization of an Imidazolium Cation by Aromatic Rings. Journal of Organic<br>Chemistry, 2022, 87, 7875-7883.                                                                                                                    | 1.7 | 2         |
| 151 | An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes<br>ChemInform, 2003, 34, no.                                                                                                                          | 0.1 | 0         |
| 152 | Discrepancy Between Common Local Aromaticity Measures in a Series of Carbazole Derivatives.<br>ChemInform, 2004, 35, no.                                                                                                                         | 0.1 | 0         |
| 153 | Theoretical Evaluation of Electron Delocalization in Aromatic Molecules by Means of Atoms in<br>Molecules (AIM) and Electron Localization Functional (ELF) Topological Approaches. ChemInform,<br>2006, 37, no.                                  | 0.1 | 0         |
| 154 | Chapter 10 Electronic structure and reactivity of aromatic metal clusters. Theoretical and Computational Chemistry, 2007, 19, 203-218.                                                                                                           | 0.2 | 0         |
| 155 | Throughâ€5pace Polarâ€Ï€ Interactions in 2,6â€Diarylthiophenols. ChemPhysChem, 2020, 21, 1080-1080.                                                                                                                                              | 1.0 | 0         |
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156 52 GAMES WITH THE PERIODIC TABLE AND BEYOND. , 2019, , .

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