## Miquel SolÃ

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/3313873/publications.pdf

Version: 2024-02-01

471 papers

20,593 citations

72 h-index

10389

20358 116 g-index

515 all docs

515 docs citations

515 times ranked 11286 citing authors

| #  | Article  | IF   | CITATIONS |
|----|--|------|-----------|
| 1  | Initiating Electron Transfer in Doubly Curved Nanographene Upon Supramolecular Complexation of $C < sub > 60 < sub > .$ Angewandte Chemie, 2022, 134, .  | 2.0  | 9         |
| 2  | Initiating Electron Transfer in Doubly Curved Nanographene Upon Supramolecular Complexation of $C < sub > 60 < / sub > .$ Angewandte Chemie - International Edition, 2022, 61, .   | 13.8 | 48        |
| 3  | Effect of Diamine Bridge on Reactivity of Tetradentate ONNO Nickel(II) Complexes. ChemPhysChem, 2022, 23, .  | 2.1  | О         |
| 4  | Enhancing the Catalytic Performance of Group I, II Metal Halides in the Cycloaddition of CO <sub>2</sub> to Epoxides under Atmospheric Conditions by Cooperation with Homogeneous and Heterogeneous Highly Nucleophilic Aminopyridines: Experimental and Theoretical Study. Journal of Organic Chemistry, 2022, 87, 2873-2886. | 3.2  | 25        |
| 5  | Path-dependency of energy decomposition analysis & Department of Land Physical Chemistry Chemical Physics, 2022, 24, 2344-2348.  | 2.8  | 27        |
| 6  | Nitrogen-doped molecular bowls as electron donors in photoinduced electron transfer reactions.<br>Nanoscale Advances, 2022, 4, 2180-2188.  | 4.6  | 6         |
| 7  | Aromaticity and Extrusion of Benzenoids Linked to [ <i>&gt;o</i> à€€OSAN] <sup>â°'</sup> : Clar Has the Answer. Angewandte Chemie - International Edition, 2022, 61, .   | 13.8 | 12        |
| 8  | Successive Diels–Alder Cycloadditions of Cyclopentadiene to [10]CPP⊃C <sub>60</sub> : A Computational Study. Journal of Organic Chemistry, 2022, 87, 5149-5157.  | 3.2  | 6         |
| 9  | Highly Selective Synthesis of Seven-Membered Azaspiro Compounds by a Rh(I)-Catalyzed<br>Cycloisomerization/Diels–Alder Cascade of 1,5-Bisallenes. Journal of Organic Chemistry, 2022, 87,<br>5279-5286.  | 3.2  | 7         |
| 10 | The importance of the bite angle of metal(III) salen catalysts in the sequestration of CO2 with epoxides in mild conditions. Green Chemical Engineering, 2022, 3, 180-187.   | 6.3  | 18        |
| 11 | Knölker Iron Catalysts for Hydrogenation Revisited: A Nonspectator Solvent and Fine-Tuning.<br>Organometallics, 2022, 41, 1204-1215.   | 2.3  | 14        |
| 12 | Three-Dimensional Fully π-Conjugated Macrocycles: When 3D-Aromatic and When 2D-Aromatic-in-3D?. Journal of the American Chemical Society, 2022, 144, 8560-8575.  | 13.7 | 28        |
| 13 | Cageâ€size effects on the encapsulation of <scp> P <sub>2</sub> </scp> by fullerenes. Journal of Computational Chemistry, 2022, , .  | 3.3  | 1         |
| 14 | The Hunter Falls Prey: Photoinduced Oxidation of C <sub>60</sub> in Inclusion Complex with Perfluorocycloparaphenylene. ChemPhysChem, 2022, 23, .  | 2.1  | 9         |
| 15 | Aromaticity of Singlet and Triplet Boron Disk-like Clusters: A Test for Electron Counting Aromaticity Rules. Inorganic Chemistry, 2022, 61, 10116-10125.   | 4.0  | 3         |
| 16 | Aromaticity rules. Nature Chemistry, 2022, 14, 585-590.  | 13.6 | 55        |
| 17 | 3D and 2D aromatic units behave like oil and water in the case of benzocarborane derivatives. Nature Communications, 2022, $13$ , .  | 12.8 | 23        |
| 18 | Mechanistic Studies of Transition-Metal-Catalyzed $[2+2+2]$ Cycloaddition Reactions. Chemical Reviews, 2021, 121, 1894-1979.   | 47.7 | 125       |

| #  | Article  | IF   | CITATIONS |
|----|--|------|-----------|
| 19 | Aromaticity of nucleic acid bases. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1509.  | 14.6 | 7         |
| 20 | Cycloaddition of CO <sub>2</sub> 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. | 4.5  | 50        |
| 21 | Aromaticity Survival in Hydrofullerenes: The Case of C 66 H 4 with Its Ï€â€Aromatic Circuits. Chemistry - A European Journal, 2021, 27, 802-808.   | 3.3  | 9         |
| 22 | An unprecedented π-electronic circuit involving an odd number of carbon atoms in a grossly warped non-planar nanographene. Chemical Communications, 2021, 57, 3087-3090.   | 4.1  | 15        |
| 23 | Photoinduced electron transfer in nano-Saturn complexes of fullerene. Physical Chemistry Chemical Physics, 2021, 23, 2126-2133.  | 2.8  | 8         |
| 24 | EXCITED-STATE AROMATICITY FOR THE DESIGN OF NEW FUNCTIONAL MATERIALS., 2021, , .   |      | 0         |
| 25 | Acenes and phenacenes in their lowest-lying triplet states. Does kinked remain more stable than straight?. Physical Chemistry Chemical Physics, 2021, 23, 13574-13582.   | 2.8  | 18        |
| 26 | Photoinduced electron transfer in mechanically interlocked suit[3]ane systems. Journal of Materials Chemistry C, 2021, 9, 9436-9445.   | 5.5  | 9         |
| 27 | The electron density of delocalized bonds (EDDBs) as a measure of local and global aromaticity. , 2021, , 259-284.   |      | 11        |
| 28 | 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.   | 1.4  | 8         |
| 29 | Guidelines for Tuning the Excited State Hückel–Baird Hybrid Aromatic Character of Proâ€Aromatic Quinoidal Compounds**. Angewandte Chemie, 2021, 133, 10343-10353.  | 2.0  | 3         |
| 30 | Guidelines for Tuning the Excited State Hýckel–Baird Hybrid Aromatic Character of Proâ€Aromatic Quinoidal Compounds**. Angewandte Chemie - International Edition, 2021, 60, 10255-10265.   | 13.8 | 17        |
| 31 | Efficient synthesis of amine-functionalized graphene oxide by ultrasound-assisted reactions and density functional theory mechanistic insight. Applied Nanoscience (Switzerland), 2021, 11, 1637-1649.   | 3.1  | 7         |
| 32 | How Do Defects in Carbon Nanostructures Regulate the Photoinduced Electron Transfer Processes? The Case of Phenine Nanotubes. ChemPhysChem, 2021, 22, 1178-1186.   | 2.1  | 7         |
| 33 | (Invited) Water-soluble fullerenes (C60 and C70) with photoinduced ROS generation. ECS Meeting Abstracts, 2021, MA2021-01, 618-618.  | 0.0  | 0         |
| 34 | Double-Carrousel Mechanism for Mn-Catalyzed Dehydrogenative Amide Synthesis from Alcohols and Amines. ACS Catalysis, 2021, 11, 6155-6161.  | 11.2 | 19        |
| 35 | Fluxional bis(phenoxy-imine) Zr and Ti catalysts for polymerization. Theoretical Chemistry Accounts, 2021, 140, 1.   | 1.4  | 2         |
| 36 | Reactivity of Li+@C60@C240 and Photoinduced Charge Shift in Li+ Doped Giant Nested Fullerenes. ECS Meeting Abstracts, 2021, MA2021-01, 635-635.  | 0.0  | 0         |

| #  | Article   | lF                     | CITATIONS    |
|----|---|------------------------|--------------|
| 37 | [10]CPPâ€Based Inclusion Complexes of Charged Fulleropyrrolidines. Effect of the Charge Location on the Photoinduced Electron Transfer. Chemistry - A European Journal, 2021, 27, 8737-8744.  | 3.3                    | 10           |
| 38 | Synthesis of Fused Dihydroazepine Derivatives of Fullerenes by a Rh atalyzed Cascade Process. Advanced Synthesis and Catalysis, 2021, 363, 3835-3844.   | 4.3                    | 8            |
| 39 | Chelation enforcing a dual gold configuration in the catalytic hydroxyphenoxylation of alkynes. Applied Organometallic Chemistry, 2021, 35, e6362.  | 3.5                    | 5            |
| 40 | Unexpected Disparity in Photoinduced Reactions of C <sub>60</sub> and C <sub>70</sub> in Water with the Generation of O <sub>2</sub> <sup><math>\hat{a} \in \hat{a} \in \langle sup \rangle \text{ or } \langle sup \rangle </math></sup> | 7.9                    | 9            |
| 41 | Predictive Catalysis in Olefin Metathesis with Ruâ€based Catalysts with Annulated C <sub>60</sub> Fullerenes in the Nâ€heterocyclic Carbenes. Chemistry - A European Journal, 2021, 27, 18074-18083.  | 3.3                    | 3            |
| 42 | Evaluation of charge-transfer rates in fullerene-based donor–acceptor dyads with different density functional approximations. Physical Chemistry Chemical Physics, 2021, 23, 5376-5384.   | 2.8                    | 18           |
| 43 | The Relative Stability of Indole Isomers Is a Consequence of the Glidewell-Lloyd Rule. Journal of Physical Chemistry A, 2021, 125, 230-234.   | 2.5                    | 16           |
| 44 | Photoinduced electron transfer in non-covalent complexes of C60 and phosphangulene oxide derivatives. Dalton Transactions, 2021, 50, 16214-16222.   | 3.3                    | 3            |
| 45 | Cage <sup>–</sup> ····Cage <sup>–</sup> Interaction: Boron Cluster-Based Noncovalent Bond and Its Applications in Solid-State Materials. Jacs Au, 2021, 1, 2047-2057.   | 7.9                    | 5            |
| 46 | Fast and Simple Evaluation of the Catalysis and Selectivity Induced by External Electric Fields. ACS Catalysis, 2021, 11, 14467-14479.  | 11.2                   | 14           |
| 47 | Reactivity of the superhalogen/superalkali ion encapsulating C <sub>60</sub> fullerenes. Dalton Transactions, 2021, 51, 203-210.  | 3.3                    | 2            |
| 48 | Cyclo[18]carbon: the smallest all-carbon electron acceptor. Chemical Communications, 2020, 56, 352-355.   | 4.1                    | 78           |
| 49 | Do Carbon Nanoâ€onions Behave as Nanoscopic Faraday Cages? A Comparison of the Reactivity of C <sub>60</sub> , C <sub>240</sub> , C <sub>60</sub> , C <sub>60</sub> , Li <sup>+</sup> , and Li <sup>+</sup> , and Li <sup>+</sup> , E <sub>60</sub> , E <sub>240</sub> . Chemistry - A European Iournal, 2020, 26, 804-808.   | 3.3                    | 12           |
| 50 | The influence of the pH on the reaction mechanism of water oxidation by a Ru(bda) catalyst. Catalysis Today, 2020, 358, 278-283.  | 4.4                    | 9            |
| 51 | Iodaneâ€Guided ortho Câ^'H Allylation. Angewandte Chemie, 2020, 132, 20376-20382.   | 2.0                    | 2            |
| 52 | Bingel–Hirsch Addition of Diethyl Bromomalonate to Ionâ€Encapsulated Fullerenes M@C 60 (M=Ã~, Li + ,) Tj ET   | QgQ 0 0 r <sub>{</sub> | gBT /Overloc |
| 53 | lodaneâ€Guided ortho Câ^'H Allylation. Angewandte Chemie - International Edition, 2020, 59, 20201-20207.  | 13.8                   | 8            |
| 54 | Probing the Origin of Adaptive Aromaticity in 16â€Valenceâ€Electron Metallapentalenes. Chemistry - A European Journal, 2020, 26, 12902-12902.   | 3.3                    | О            |

| #  | Article  | IF           | CITATIONS |
|----|--|--------------|-----------|
| 55 | Understanding the performance of a bisphosphonate Ru water oxidation catalyst. Dalton Transactions, 2020, 49, 14052-14060.   | 3.3          | 10        |
| 56 | All-metal Baird aromaticity. Chemical Communications, 2020, 56, 12522-12525.   | 4.1          | 25        |
| 57 | Photoinduced electron transfer in nanotube $\hat{S}_fC$ (sub>70 inclusion complexes: phenine (i>vsnanographene nanotubes. Chemical Communications, 2020, 56, 12624-12627.  | 4.1          | 16        |
| 58 | Electron Transfer in a Li∢sup>+∢/sup>-Doped Zn-Porphyrin–[10]CPPâŠ∱Fullerene Junction and Charge-Separated Bands with Opposite Response to Polar Environments. Journal of Physical Chemistry B, 2020, 124, 9095-9102.  | 2.6          | 16        |
| 59 | Covalent Functionalization of Single-Walled Carbon Nanotubes by the Bingel Reaction for Building Charge-Transfer Complexes. Journal of Organic Chemistry, 2020, 85, 11721-11731.   | 3.2          | 6         |
| 60 | 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.   | 2.8          | 12        |
| 61 | Triquinoline―versus Fullereneâ€Based Cycloparaphenylene Ionic Complexes: Comparison of Photoinduced Chargeâ€Shift Reactions. Chemistry - A European Journal, 2020, 26, 10896-10902.  | 3.3          | 10        |
| 62 | Substituted adenine quartets: interplay between substituent effect, hydrogen bonding, and aromaticity. RSC Advances, 2020, 10, 23350-23358.  | 3.6          | 6         |
| 63 | Mechanism of the Facile Nitrous Oxide Fixation by Homogeneous Ruthenium Hydride Pincer Catalysts.<br>Inorganic Chemistry, 2020, 59, 9374-9383.   | 4.0          | 14        |
| 64 | Probing the Origin of Adaptive Aromaticity in 16â€Valenceâ€Electron Metallapentalenes. Chemistry - A European Journal, 2020, 26, 12964-12971.  | 3.3          | 28        |
| 65 | Effect of Alkali Metal Cations on Length and Strength of Hydrogen Bonds in DNA Base Pairs.<br>ChemPhysChem, 2020, 21, 2112-2126.   | 2.1          | 15        |
| 66 | The nido â€Cageâ‹â‹â‹ï€ Bond: A Nonâ€covalent Interaction between Boron Clusters and Aromatic Rings and Applications. Angewandte Chemie, 2020, 132, 9103-9110.   | d lts<br>2.0 | 7         |
| 67 | The <i>nido</i> â€Cageâââï€ Bond: A Nonâ€covalent Interaction between Boron Clusters and Aromatic Rin<br>and Its Applications. Angewandte Chemie - International Edition, 2020, 59, 9018-9025.   | ngs<br>13.8  | 32        |
| 68 | 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.  | 2.5          | 4         |
| 69 | Too Persistent to Give Up: Aromaticity in Boron Clusters Survives Radical Structural Changes.<br>Journal of the American Chemical Society, 2020, 142, 9396-9407.   | 13.7         | 145       |
| 70 | (Invited) Reactivity of Li+@C60@C240 and Photoinduced Charge Shift in Li+ Doped Giant Nested Fullerenes. ECS Meeting Abstracts, 2020, MA2020-01, 809-809.  | 0.0          | 0         |
| 71 | (Invited) Preparation of Open-Cage Fullerene Derivatives By Rhodium(I)-Catalyzed [2+2+2]<br>Cycloaddition of Diynes and C60: Synthesis, Computational Studies and Application in Perovskite Solar<br>Cells. ECS Meeting Abstracts, 2020, MA2020-01, 786-786. | 0.0          | O         |
| 72 | A Rh-Catalyzed Cycloisomerization/Diels–Alder Cascade Reaction of 1,5-Bisallenes for the Synthesis of Polycyclic Heterocycles. Organic Letters, 2019, 21, 6608-6613.   | 4.6          | 18        |

| #  | Article  | IF   | CITATIONS |
|----|--|------|-----------|
| 73 | Examining the Factors That Govern the Regioselectivity in Rhodium-Catalyzed Alkyne Cyclotrimerization. Organometallics, 2019, 38, 2853-2862.   | 2.3  | 34        |
| 74 | Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.  | 3.3  | 113       |
| 75 | Special Collection: Computational Chemistry. ChemistryOpen, 2019, 8, 814-816.  | 1.9  | 3         |
| 76 | Mechanism of the Manganese-Pincer-Catalyzed Acceptorless Dehydrogenative Coupling of Nitriles and Alcohols. Journal of the American Chemical Society, 2019, 141, 2398-2403.                          | 13.7 | 69        |
| 77 | Hypsochromic solvent shift of the charge separation band in ionic donor–acceptor<br>Li <sup>+</sup> @C <sub>60</sub> âŠ,[10]CPP. Chemical Communications, 2019, 55, 11195-11198.                     | 4.1  | 23        |
| 78 | Exploiting the Aromatic Chameleon Character of Fulvenes for Computational Design of Bairdâ€Aromatic Triplet Ground State Compounds. Chemistry - an Asian Journal, 2019, 14, 1870-1878.               | 3.3  | 13        |
| 79 | Regioselectivity in Diels–Alder Cycloadditions of #6094C68 Fullerene with a Triplet Ground State.<br>Journal of Organic Chemistry, 2019, 84, 9017-9024.  | 3.2  | 7         |
| 80 | Photoinduced Charge Shift in Li <sup>+</sup> -Doped Giant Nested Fullerenes. Journal of Physical Chemistry C, 2019, 123, 16525-16532.  | 3.1  | 13        |
| 81 | Effect of Exocyclic Substituents and π-System Length on the Electronic Structure of Chichibabin Diradical(oid)s. ACS Omega, 2019, 4, 10845-10853.  | 3.5  | 10        |
| 82 | Innenrù⁄4cktitelbild: Allâ€Fullerene Electron Donor–Acceptor Conjugates (Angew. Chem. 21/2019).<br>Angewandte Chemie, 2019, 131, 7217-7217.  | 2.0  | 1         |
| 83 | Allâ€Fullerene Electron Donor–Acceptor Conjugates. Angewandte Chemie - International Edition, 2019, 58, 6932-6937.   | 13.8 | 35        |
| 84 | Is Excitedâ€State Aromaticity a Driving Force for Planarization of Dibenzannelated 8Ï€â€Electron Heterocycles?. ChemPlusChem, 2019, 84, 712-721.   | 2.8  | 38        |
| 85 | Allâ€Fullerene Electron Donor–Acceptor Conjugates. Angewandte Chemie, 2019, 131, 7006-7011.  | 2.0  | 13        |
| 86 | Electron Delocalization in Planar Metallacycles: Hýckel or Möbius Aromatic?. ChemistryOpen, 2019, 8, 219-227.  | 1.9  | 49        |
| 87 | The Coulomb Hole of the Ne Atom. ChemistryOpen, 2019, 8, 411-417.  | 1.9  | 6         |
| 88 | Open-shell jellium aromaticity in metal clusters. Chemical Communications, 2019, 55, 5559-5562.  | 4.1  | 15        |
| 89 | Decomposition of the electronic activity in competing [5,6] and [6,6] cycloaddition reactions between C <sub>60</sub> and cyclopentadiene. Physical Chemistry Chemical Physics, 2019, 21, 5039-5048. | 2.8  | 11        |
| 90 | Photoinduced electron transfer and unusual environmental effects in fullerene–Zn-porphyrin–BODIPY triads. Physical Chemistry Chemical Physics, 2019, 21, 25098-25107.                                | 2.8  | 22        |

| #   | Article  | IF           | CITATIONS |
|-----|--|--------------|-----------|
| 91  | Tuning the Strength of the Resonance-Assisted Hydrogen Bond in Acenes and Phenacenes with Two ⟨i>o⟨ i>-Hydroxyaldehyde Groupsâ€"The Importance of Topology. Journal of Organic Chemistry, 2019, 84, 15538-15548. | 3.2          | 13        |
| 92  | Connecting and combining rules of aromaticity. Towards a unified theory of aromaticity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1404.  | 14.6         | 37        |
| 93  | Peculiar Photoinduced Electron Transfer in Porphyrin–Fullerene Akamptisomers. Chemistry - A<br>European Journal, 2019, 25, 2577-2585.  | 3.3          | 9         |
| 94  | (Invited) Photoinduced Charge Separation in Several Dyads Involving Fullerenes. ECS Meeting Abstracts, 2019, , .   | 0.0          | 0         |
| 95  | 52 GAMES WITH THE PERIODIC TABLE AND BEYOND., 2019,,.  |              | 0         |
| 96  | Rationalizing the Regioselectivity of the Diels–Alder Biscycloaddition of Fullerenes. Journal of Organic Chemistry, 2018, 83, 3285-3292.   | 3.2          | 11        |
| 97  | Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. Chemistry - A European Journal, 2018, 24, 9853-9859.   | 3.3          | 28        |
| 98  | Reliable charge assessment on encapsulated fragment for endohedral systems. Scientific Reports, 2018, 8, 2882.   | 3.3          | 5         |
| 99  | Tuning the Strength of the Resonance-Assisted Hydrogen Bond in <i>o</i> -Hydroxybenzaldehyde by Substitution in the Aromatic Ring <sup>1</sup> . Journal of Physical Chemistry A, 2018, 122, 2279-2287.          | 2.5          | 28        |
| 100 | On the regioselectivity of the Diels–Alder cycloaddition to C <sub>60</sub> in high spin states. Physical Chemistry Chemical Physics, 2018, 20, 11577-11585.   | 2.8          | 10        |
| 101 | Electron-Pair Distribution in Chemical Bond Formation. Journal of Physical Chemistry A, 2018, 122, 1916-1923.  | 2.5          | 6         |
| 102 | Aromaticity of acenes: the model of migrating π-circuits. Physical Chemistry Chemical Physics, 2018, 20, 13430-13436.  | 2.8          | 36        |
| 103 | Mechanism of the Selective Fe-Catalyzed Arene Carbon–Hydrogen Bond Functionalization. ACS Catalysis, 2018, 8, 4313-4322.   | 11.2         | 32        |
| 104 | Influence of the charge on the reactivity of azafullerenes. Physical Chemistry Chemical Physics, 2018, 20, 28011-28018.  | 2.8          | 11        |
| 105 | Aromaticity Determines the Relative Stability of Kinked vs. Straight Topologies in Polycyclic Aromatic Hydrocarbons. Frontiers in Chemistry, 2018, 6, 561.   | 3.6          | 41        |
| 106 | Stereocontrolled Photoinduced Electron Transfer in Metalâ€Fullerene Hybrids. Chemistry - A European Journal, 2018, 24, 13020-13025.  | 3.3          | 17        |
| 107 | Regioselectivity of the Pauson–Khand reaction in single-walled carbon nanotubes. Nanoscale, 2018, 10, 15078-15089.   | 5 <b>.</b> 6 | 11        |
| 108 | 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.   | 3.3          | 0         |

| #   | Article   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 109 | 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, 1974.                                      | 4.1 | 14        |
| 110 | The electronic structure and stability of germanium tubes Ge <sub>30</sub> H <sub>12</sub> and Ge <sub>33</sub> H <sub>12</sub> . Physical Chemistry Chemical Physics, 2018, 20, 23467-23479.                                 | 2.8 | 6         |
| 111 | Expeditious Preparation of Openâ€Cage Fullerenes by Rhodium(I)â€Catalyzed [2+2+2] Cycloaddition of Diynes and C <sub>60</sub> : An Experimental and Theoretical Study. Chemistry - A European Journal, 2018, 24, 10653-10661. | 3.3 | 28        |
| 112 | Tuning diastereoisomerism in platinum(ii) phosphino- and aminothiolato hydrido complexes. New Journal of Chemistry, 2017, 41, 3015-3028.  | 2.8 | 1         |
| 113 | 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.   | 3.3 | 71        |
| 114 | Is coronene better described by <scp>C</scp> lar's aromatic Ï€â€sextet model or by the AdNDP representation?. Journal of Computational Chemistry, 2017, 38, 1606-1611.  | 3.3 | 30        |
| 115 | The role of the longâ€range exchange corrections in the description of electron delocalization in aromatic species. Journal of Computational Chemistry, 2017, 38, 1640-1654.  | 3.3 | 69        |
| 116 | Understanding the Reactivity of Ionâ€Encapsulated Fullerenes. Chemistry - A European Journal, 2017, 23, 11030-11036.  | 3.3 | 33        |
| 117 | Can Baird's and Clar's Rules Combined Explain Triplet State Energies of Polycyclic Conjugated Hydrocarbons with Fused 4 <i>n</i>  i> i∈- and (4 <i>n</i> + 2) i∈-Rings?. Journal of Organic Chemistry, 2017, 82, 6327-6340.   | 3.2 | 55        |
| 118 | Mechanism of the Suzuki–Miyaura Cross-Coupling Reaction Mediated by [Pd(NHC)(allyl)Cl] Precatalysts. Organometallics, 2017, 36, 2088-2095.  | 2.3 | 68        |
| 119 | Rationalizing the relative abundances of trimetallic nitride template-based endohedral metallofullerenes from aromaticity measures. Chemical Communications, 2017, 53, 4140-4143.   | 4.1 | 5         |
| 120 | Predicting and Understanding the Reactivity of Aza[60]fullerenes. Journal of Organic Chemistry, 2017, 82, 754-758.  | 3.2 | 20        |
| 121 | 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.         | 2.8 | 9         |
| 122 | The electron density of delocalized bonds (EDDB) applied for quantifying aromaticity. Physical Chemistry Chemical Physics, 2017, 19, 28970-28981.   | 2.8 | 114       |
| 123 | A Computational Study of the Intermolecular [2+2+2] Cycloaddition of Acetylene and C <sub>60</sub> Catalyzed by Wilkinson's Catalyst. Chemistry - A European Journal, 2017, 23, 15067-15072.                                  | 3.3 | 11        |
| 124 | Does the endohedral borospherene supersalt FLi <sub>2</sub> @B <sub>39</sub> maintain the "super― properties of its subunits?. Physical Chemistry Chemical Physics, 2017, 19, 21276-21281.                                    | 2.8 | 6         |
| 125 | The key role of aromaticity in the structure and reactivity of C60 and endohedral metallofullerenes. Inorganica Chimica Acta, 2017, 468, 38-48.   | 2.4 | 8         |
| 126 | Rhodium atalyzed [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.                           | 3.3 | 22        |

| #   | Article  | IF         | CITATIONS    |
|-----|--|------------|--------------|
| 127 | Unusual reactivity of rhodium carbenes with allenes: an efficient asymmetric synthesis of methylenetetrahydropyran scaffolds. Chemical Communications, 2017, 53, 9922-9925.  | 4.1        | 15           |
| 128 | Effect of incarcerated HF on the exohedral chemical reactivity of HF@C <sub>60</sub> . Chemical Communications, 2017, 53, 10993-10996.   | 4.1        | 26           |
| 129 | Why Aromaticity Is a Suspicious Concept? Why?. Frontiers in Chemistry, 2017, 5, 22.  | 3.6        | 108          |
| 130 | Theoretical estimation of the rate of photoinduced charge transfer reactions in triphenylamine C <sub>60</sub> donor–acceptor conjugate. Journal of Computational Chemistry, 2016, 37, 1396-1405.  | 3.3        | 10           |
| 131 | Reactivity and Selectivity of Bowlâ€Shaped Polycyclic Aromatic Hydrocarbons: Relationship to C <sub>60</sub> . Chemistry - A European Journal, 2016, 22, 1368-1378.  | 3.3        | 31           |
| 132 | In Silico Olefin Metathesis with Ruâ€Based Catalysts Containing Nâ€Heterocyclic Carbenes Bearing C <sub>60</sub> Fullerenes. Chemistry - A European Journal, 2016, 22, 6617-6623.  | 3.3        | 15           |
| 133 | Understanding the Reactivity of Planar Polycyclic Aromatic Hydrocarbons: Towards the Graphene<br>Limit. Chemistry - A European Journal, 2016, 22, 10572-10580.   | 3.3        | 27           |
| 134 | Photoinduced Charge Separation in the Carbon Nano-Onion C <sub>60</sub> @C <sub>240</sub> . Journal of Physical Chemistry A, 2016, 120, 5798-5804.   | 2.5        | 10           |
| 135 | Reaction Mechanism and Regioselectivity of the Bingel–Hirsch Addition of Dimethyl Bromomalonate to La@ <i>C</i> <sub>2<i>v</i></sub> <sub>82</sub> . Chemistry - A European Journal, 2016, 22, 5953-5962.                                      | 3.3        | 23           |
| 136 | The Regioselectivity of Bingel–Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie, 2016, 128, 2420-2423.  | 2.0        | 9            |
| 137 | Celebrating the $150 \mathrm{th}$ anniversary of the Kekul $	ilde{A}$ benzene structure. Physical Chemistry Chemical Physics, $2016,18,11587$ - $11588.$   | 2.8        | 26           |
| 138 | Rules of Aromaticity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 321-335.   | 0.6        | 7            |
| 139 | Structural Preferences in Phosphanylthiolato Platinum(II) Complexes. ChemistryOpen, 2016, 5, 51-59.  | 1.9        | 6            |
| 140 | Planar <i>vs. </i> three-dimensional X <sub>6</sub> <sup>2â^'</sup> , 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, Physical Chemistry Chemical Physics, 2016, 18, 21102-21110. | ) Tj.ETQq0 | 0,0 rgBT /O\ |
| 141 | The Driving Force of Photoinduced Charge Separation in Metalâ€Clusterâ€Encapsulated Triphenylamineâ€[80]fullerenes. Chemistry - A European Journal, 2016, 22, 17305-17310.   | 3.3        | 5            |
| 142 | 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.   | 1.4        | 24           |
| 143 | The Regioselectivity of Bingel–Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie - International Edition, 2016, 55, 2374-2377.   | 13.8       | 37           |
| 144 | Analysis of a Compound Class with Triplet States Stabilized by Potentially Baird Aromatic [10]Annulenyl Dicationic Rings. Chemistry - A European Journal, 2016, 22, 2793-2800.   | 3.3        | 30           |

| #   | Article  | IF         | CITATIONS                  |
|-----|--|------------|----------------------------|
| 145 | Hýckel's Rule of Aromaticity Categorizes Aromatic <i>closo</i> Boron Hydride Clusters. Chemistry - A European Journal, 2016, 22, 7437-7443.  | 3.3        | 103                        |
| 146 | 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.  | 3.3        | 10                         |
| 147 | Fmocâ€"RGDS based fibrils: atomistic details of their hierarchical assembly. Physical Chemistry Chemical Physics, 2016, 18, 1265-1278.   | 2.8        | 17                         |
| 148 | Octahedral aromaticity in $\langle sup \rangle 2S + 1 \langle sup \rangle A \langle sub \rangle 1g \langle sub \rangle X \langle sub \rangle 6 \langle sub \rangle \langle sup \rangle q \langle sup \rangle clusters (X =) Tj ET (Sup Sup Sup Sup Sup Sup Sup Sup Sup Sup $ | Qq0 0 0 rg | gBT <sub>12</sub> Overlock |
| 149 | Bonding description of the Harpoon mechanism. Molecular Physics, 2016, 114, 1345-1355.   | 1.7        | 13                         |
| 150 | Structural Preferences in Phosphanylthiolato Platinum(II) Complexes. ChemistryOpen, 2016, 5, 2-2.  | 1.9        | 1                          |
| 151 | (4+2) and $(2+2)$ Cycloadditions of Benzyne to C <sub>60</sub> and Zig-Zag Single-Walled Carbon Nanotubes: The Effect of the Curvature. Journal of Physical Chemistry C, 2016, 120, 1716-1726.   | 3.1        | 34                         |
| 152 | Nitrite to nitric oxide interconversion by heme Fell complex assisted by [Cul(tmpa)]+. Structural Chemistry, 2016, 27, 409-417.  | 2.0        | 3                          |
| 153 | (Invited) The Regioselectivity of the Diels-Alder and Bingel-Hirsch Additions to La@C2 $\nu$ -C82. ECS Meeting Abstracts, 2016, , .  | 0.0        | 0                          |
| 154 | (Invited) Photoinduced Charge Transfer Reactions and Excited State Properties in Triphenylamine C60 Donor-Acceptor Conjugates. ECS Meeting Abstracts, 2016, , .  | 0.0        | 0                          |
| 155 | (Invited) Aromaticity, Cage Structure, and Relative Abundancy of Endohedral Metallofullerenes. ECS Meeting Abstracts, 2016, , .  | 0.0        | 0                          |
| 156 | (Invited) The Regioselectivity of Bingel-Hirsch Cycloadditions on IPR Endohedral Metallofullerenes. ECS Meeting Abstracts, $2016$ , , .  | 0.0        | 0                          |
| 157 | Enantioselective Rhodium(I) Donor Carbenoidâ€Mediated Cascade Triggered by a Baseâ€Free Decomposition of Arylsulfonyl Hydrazones. Chemistry - A European Journal, 2015, 21, 16240-16245.   | 3.3        | 37                         |
| 158 | On the Reaction Mechanism of the Rhodium-Catalyzed Arylation of Fullerene (C <sub>60</sub> ) with Organoboron Compounds in the Presence of Water. ChemistryOpen, 2015, 4, 774-778.   | 1.9        | 12                         |
| 159 | Enantiospecific <i>cis</i> â€" <i>trans</i> Isomerization in Chiral Fulleropyrrolidines:<br>Hydrogen-Bonding Assistance in the Carbanion Stabilization in H <sub>2</sub> 0@C <sub>60</sub> .<br>Journal of the American Chemical Society, 2015, 137, 1190-1197.              | 13.7       | 40                         |
| 160 | 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.                                     | 1.4        | 13                         |
| 161 | Acidic C–H Bond as a Proton Donor in Excited State Intramolecular Proton Transfer Reactions. Journal of Chemical Theory and Computation, 2015, 11, 1046-1054.  | 5.3        | 65                         |
| 162 | Three-center bonding analyzed from correlated and uncorrelated third-order reduced density matrices. Computational and Theoretical Chemistry, 2015, 1053, 173-179.   | 2.5        | 8                          |

| #   | Article   | IF                      | Citations     |
|-----|---|-------------------------|---------------|
| 163 | On the existence and characterization of molecular electrides. Chemical Communications, 2015, 51, 4865-4868.  | 4.1                     | 68            |
| 164 | Understanding the Reactivity of Endohedral Metallofullerenes: C <sub>78</sub> versus Sc <sub>3</sub> N@C <sub>78</sub> . Chemistry - A European Journal, 2015, 21, 5760-5768.                               | 3.3                     | 45            |
| 165 | The Missing Entry in the Agostic–Anagostic Series: Rh(I)–η <sup>1</sup> -C Interactions in P(CH)P Pincer Complexes. Inorganic Chemistry, 2015, 54, 2960-2969.   | 4.0                     | 46            |
| 166 | Why 1,2-quinone derivatives are more stable than their 2,3-analogues?. Theoretical Chemistry Accounts, 2015, 134, 1.  | 1.4                     | 16            |
| 167 | Quantifying aromaticity with electron delocalisation measures. Chemical Society Reviews, 2015, 44, 6434-6451.   | 38.1                    | 335           |
| 168 | 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, 8223-8236.                     | 4.0                     | 24            |
| 169 | Reusable manganese compounds containing pyrazole-based ligands for olefin epoxidation reactions. Dalton Transactions, 2015, 44, 17529-17543.  | 3.3                     | 18            |
| 170 | A theoretical study of the aromaticity in neutral and anionic borole compounds. Dalton Transactions, 2015, 44, 6740-6747.   | 3.3                     | 37            |
| 171 | Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.  | 2.5                     | 99            |
| 172 | Understanding the Exohedral Functionalization of Endohedral Metallofullerenes Metallofullerenes. Carbon Materials, 2015, , 67-99.   | 1.2                     | 0             |
| 173 | Computational insight into Wilkinson's complex catalyzed [2Â+Â2Â+Â2] cycloaddition mechanism leading to pyridine formation. Journal of Organometallic Chemistry, 2014, 768, 15-22.                          | 1.8                     | 15            |
| 174 | Exploring the Potential Energy Surface of E <sub>2</sub> P <sub>4</sub> Clusters (E=Groupâ€13 Element): The Quest for Inverse Carbonâ€Free Sandwiches. Chemistry - A European Journal, 2014, 20, 4583-4590. | 3.3                     | 19            |
| 175 | Stereoselective Rhodiumâ€Catalysed [2+2+2] Cycloaddition of Linear Allene–Ene/Yne–Allene Substrates: Reactivity and Theoretical Mechanistic Studies. Chemistry - A European Journal, 2014, 20, 5034-5045.   | 3.3                     | 37            |
| 176 | Origin of Reactivity Trends of Noble Gas Endohedral Fullerenes Ng <sub>2</sub> @C <sub>60</sub> (Ng) Tj ETQq  | <sub>1</sub> 0 0 0 rgB⊺ | T/gyerlock 10 |
| 177 | A new mild synthetic route to N-arylated pyridazinones from aryldiazonium salts. Chemical Communications, 2014, 50, 8073-8076.  | 4.1                     | 6             |
| 178 | Ï€â€Aromaticity and Threeâ€Dimensional Aromaticity: Two sides of the Same Coin?. Angewandte Chemie - International Edition, 2014, 53, 12191-12195.  | 13.8                    | 242           |
| 179 | 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.                      | 3.1                     | 15            |
|     |   |                         | -             |

The role of aromaticity in determining the molecular structure and reactivity of (endohedral) Tj ETQq0.00 rgBT /Ovgrlqck 10.75 ft 50.62 Td 97 ft 10.75 ft

11

180

| #   | Article  | IF                           | CITATIONS              |
|-----|--|------------------------------|------------------------|
| 181 | Electroactive polymers for the detection of morphine. Journal of Polymer Research, 2014, 21, 1.  | 2.4                          | 6                      |
| 182 | Aromaticity and Magnetic Properties of 1―and 2â€Indenones and Their Aza Derivatives. European Journal of Organic Chemistry, 2014, 2014, 5370-5377.   | 2.4                          | 9                      |
| 183 | Analysis of the Aromaticity of Five-Membered Heterometallacycles Containing Os, Ru, Rh, and Ir. Organometallics, 2014, 33, 1762-1773.  | 2.3                          | 31                     |
| 184 | New Approximation to the Third-Order Density. Application to the Calculation of Correlated Multicenter Indices. Journal of Chemical Theory and Computation, 2014, 10, 3055-3065.   | <b>5.</b> 3                  | 31                     |
| 185 | Dinuclear Ru–Aqua Complexes for Selective Epoxidation Catalysis Based on Supramolecular Substrate Orientation Effects. Chemistry - A European Journal, 2014, 20, 3898-3902.  | 3.3                          | 32                     |
| 186 | Aromatic properties of 8-hydroxyquinoline and its metal complexes. Open Chemistry, 2013, 11, 655-663.  | 1.9                          | 8                      |
| 187 | Aromaticity as the driving force for the stability of non-IPR endohedral metallofullerene<br>Bingel–Hirsch adducts. Chemical Communications, 2013, 49, 8767.   | 4.1                          | 21                     |
| 188 | Maximum Aromaticity as a Guiding Principle for the Most Suitable Hosting Cages in Endohedral Metallofullerenes. Angewandte Chemie - International Edition, 2013, 52, 9275-9278.  | 13.8                         | 55                     |
| 189 | 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.  | 2.5                          | 9                      |
| 190 | Unraveling the Origin of the Relative Stabilities of Group 14 $M$ <sub>2</sub> N <sub>2</sub> <sup>2+</sup> (M, N = C, Si, Ge, Sn, and Pb) Isomer Clusters. Journal of Physical Chemistry A, 2013, 117, 10462-10469.   | 2.5                          | 13                     |
| 191 | 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.   | 2.6                          | 6                      |
| 192 | $X \cdot sub \cdot 2 \cdot  sub \cdot Y \cdot sub \cdot 2 \cdot  sub \cdot Stability  sub \cdot 2 \cdot  $ | 4.0                          | 16                     |
| 193 | A Complete Guide on the Influence of Metal Clusters in the Diels–Alder Regioselectivity of <i>I<sub>h</sub></i> i>1 <sub>h</sub> i>14931-14940.  | 3.3                          | 37                     |
| 194 | Analysis of the Relative Stabilities of Ortho, Meta, and Para MCIY(XC <sub>4</sub> H <sub>4</sub> )(PH <sub>3</sub> ) <sub>2</sub> Heterometallabenzenes (M = Rh,) Tj E  | :T <b>Q¤<sub>1</sub>3</b> 00 | rg <b>B</b> i6/Overloc |
| 195 | Examining the formation of specific interactions between poly(3,4-ethylenedioxythiophene) and nucleotide bases. RSC Advances, 2013, 3, 2639.   | 3.6                          | 7                      |
| 196 | Electrochemical control of the regioselectivity in the exohedral functionalization of C60: the role of aromaticity. Chemical Communications, 2013, 49, 1220.   | 4.1                          | 44                     |
| 197 | Metalloaromaticity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 105-122.  | 14.6                         | 105                    |
| 198 | Diels–Alder and Retroâ€Diels–Alder Cycloadditions of (1,2,3,4,5â€Pentamethyl)cyclopentadiene to La@ <i>C</i> < <sub>2<i>v</i></sub> â€C <sub>82</sub> : Regioselectivity and Product Stability. Chemistry - A European Journal, 2013, 19, 4468-4479.   | 3.3                          | 27                     |

| #   | Article   | lF  | Citations |
|-----|---|-----|-----------|
| 199 | A Simple Link between Hydrocarbon and Borohydride Chemistries. Chemistry - A European Journal, 2013, 19, 4169-4175.   | 3.3 | 40        |
| 200 | Why Do Cycloaddition Reactions Involving C <sub>60</sub> Prefer [6,6] over [5,6] Bonds?. Chemistry - A European Journal, 2013, 19, 7416-7422.   | 3.3 | 100       |
| 201 | Ruthenium Complexes with Chiral Bis-Pinene Ligands: an Array of Subtle Structural Diversity.<br>Inorganic Chemistry, 2013, 52, 4985-4992.   | 4.0 | 7         |
| 202 | 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 | 5         |
| 203 | On the Validity of the Maximum Hardness Principle and the Minimum Electrophilicity Principle during Chemical Reactions. Journal of Physical Chemistry A, 2013, 117, 1843-1852.  | 2.5 | 152       |
| 204 | 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, 520-532.                               | 5.3 | 9         |
| 205 | Nâ€Tetradentate SPANamine Derivatives and Their Mn <sup>II</sup> omplexes as Catalysts for Epoxidation of Alkenes. European Journal of Inorganic Chemistry, 2013, 2013, 1213-1224.  | 2.0 | 19        |
| 206 | Forty years of Clar's aromatic π-sextet rule. Frontiers in Chemistry, 2013, 1, 22.  | 3.6 | 332       |
| 207 | Complete $\ddot{l}f^*$ intramolecular aromatic hydroxylation mechanism through O2 activation by a Schiff base macrocyclic dicopper(I) complex. Beilstein Journal of Organic Chemistry, 2013, 9, 585-593.                                | 2.2 | 6         |
| 208 | Tuning the Electronic Properties by Width and Length Modifications of Narrow-Diameter Carbon Nanotubes for Nanomedicine. Current Medicinal Chemistry, 2012, 19, 5219-5225.  | 2.4 | 17        |
| 209 | A new DFT functional based on spin-states and SN2 barriers. , 2012, , .   |     | 0         |
| 210 | Molecular structures of M2N22 $\hat{a}$ (M and N = B, Al, and Ga) clusters using the gradient embedded genetic algorithm. Physical Chemistry Chemical Physics, 2012, 14, 14850.   | 2.8 | 18        |
| 211 | On the electronic structure of second generation Hoveyda–Grubbs alkene metathesis precursors.<br>Computational and Theoretical Chemistry, 2012, 996, 57-67.   | 2.5 | 21        |
| 212 | Product formation in the Prato reaction on Sc3N@D5h-C80: preference for [5,6]-bonds, and not pyracylenic bonds. Chemical Communications, 2012, 48, 2486.  | 4.1 | 26        |
| 213 | Properties of poly(3-halidethiophene)s. Physical Chemistry Chemical Physics, 2012, 14, 10050.   | 2.8 | 8         |
| 214 | 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, 1671-1683. | 5.3 | 18        |
| 215 | Direct Detection of Key Intermediates in Rhodium(I) atalyzed [2+2+2] Cycloadditions of Alkynes by ESIâ€MS. Chemistry - A European Journal, 2012, 18, 13097-13107.   | 3.3 | 37        |
| 216 | The linear response kernel of conceptual DFT as a measure of aromaticity. Physical Chemistry Chemical Physics, 2012, 14, 3960.  | 2.8 | 51        |

| #   | Article   | lF          | Citations |
|-----|---|-------------|-----------|
| 217 | Electronic and Vibrational Nonlinear Optical Properties of Five Representative Electrides. Journal of Chemical Theory and Computation, 2012, 8, 2688-2697.  | <b>5.</b> 3 | 78        |
| 218 | On the reliability of the maximum hardness and minimum polarizability principles in nontotally symmetric vibrations. , 2012, , .  |             | 1         |
| 219 | The Exonedral Dielsa€ Alder Reactivity of the Titanium Carbide Endonedral Metallorullerene Ti <sub>2</sub> C <sub>2</sub> @ <i>D</i> <sub>3<i>h</i><sub>â€C<sub>78</sub>?6<csub>78</csub></sub> and M<sub>3</sub>N@<i>D</i><sub>3<i>h</i><fi>h<fi>h<fi>h</fi></fi></fi></sub>3<fi>h<fi>h</fi></fi></sub> 3 <fi>h3</fi> <fi>h3</fi> <fi>h6</fi> <fi>h6</fi> <fi>h78</fi> <fi>h78<fi>h78hh<td< td=""><td>3.3</td><td>54</td></td<></fi></fi> | 3.3         | 54        |
| 220 | Full Exploration of the Diels–Alder Cycloaddition on Metallofullerenes M <sub>3</sub> N@C <sub>80</sub> (M=Sc, Lu, Gd): The <i>D</i> <sub>5<i>h</i></sub> Versus <i>l<sub>h</sub></i> Isomer and the Influence of the Metal Cluster. Chemistry - A European Journal, 2012, 18, 8944-8956.   | 3.3         | 49        |
| 221 | Open-shell spherical aromaticity: the 2N2 + 2N + 1 (with S = N + $\hat{A}^{1/2}$ ) rule. Chemical Communications, 2011, 47, 11647.  | 4.1         | 49        |
| 222 | A donor-functionalized, silyl-substituted pentadienyllithium: structural insight from experiment and theory. Chemical Communications, 2011, 47, 6162.   | 4.1         | 14        |
| 223 | Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2011, 7, 1231-1231.  | 5.3         | 7         |
| 224 | Nuclear Shieldings with the SSB-D Functional. Journal of Physical Chemistry A, 2011, 115, 1250-1256.  | 2.5         | 16        |
| 225 | RhCl(PPh <sub>3</sub> ) <sub>3</sub> -Catalyzed Intramolecular Cycloaddition of Enediynes: The Nature of the Tether and Substituents Controls the Reaction Mechanism. Organometallics, 2011, 30, 3151-3159.   | 2.3         | 22        |
| 226 | New Ru(II) Complexes Containing Oxazoline Ligands As Epoxidation Catalysts. Influence of the Substituents on the Catalytic Performance. Inorganic Chemistry, 2011, 50, 6044-6054.   | 4.0         | 30        |
| 227 | All-metal aromatic clusters M42â^' (M = B, Al, and Ga). Are Ï€-electrons distortive or not?. Physical Chemistry Chemical Physics, 2011, 13, 20673.  | 2.8         | 14        |
| 228 | DFT Study of Thermal 1,3-Dipolar Cycloaddition Reactions between Alkynyl Metal(0) Fischer Carbene Complexes and 3 <i>H</i> -1,2-Dithiole-3-thione Derivatives. Organometallics, 2011, 30, 466-476.  | 2.3         | 38        |
| 229 | Understanding Conjugation and Hyperconjugation from Electronic Delocalization Measures. Journal of Physical Chemistry A, 2011, 115, 13104-13113.  | 2.5         | 30        |
| 230 | The reactivity of endohedral fullerenes. What can be learnt from computational studies?. Physical Chemistry Chemical Physics, 2011, 13, 3585-3603.  | 2.8         | 128       |
| 231 | Routes of Ï∈-Electron Delocalization in 4-Substituted-1,2-benzoquinones. Journal of Organic Chemistry, 2011, 76, 550-556.   | 3.2         | 15        |
| 232 | 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.  | 3.2         | 43        |
| 233 | Dispersion Corrections Essential for the Study of Chemical Reactivity in Fullerenes. Journal of Physical Chemistry A, 2011, 115, 3491-3496.   | 2.5         | 117       |
| 234 | Binding of 6-mer single-stranded homo-nucleotides to poly(3,4-ethylenedioxythiophene): specific hydrogen bonds with guanine. Soft Matter, 2011, 7, 9922.  | 2.7         | 13        |

| #   | Article   | IF               | CITATIONS  |
|-----|---|------------------|------------|
| 235 | Organomagnesium clusters: Structure, stability, and bonding in archetypal models. Journal of Organometallic Chemistry, 2011, 696, 4104-4111.  | 1.8              | 13         |
| 236 | Ab Initio Design of Chelating Ligands Relevant to Alzheimer's Disease: Influence of Metalloaromaticity. Journal of Physical Chemistry A, 2011, 115, 12659-12666.  | 2.5              | 20         |
| 237 | Analysis of the Effects of N-Substituents on Some Aspects of the Aromaticity of Imidazoles and Pyrazoles. Journal of Physical Chemistry A, 2011, 115, 8571-8577.  | 2.5              | 46         |
| 238 | Nucleophilic Aryl Fluorination and Aryl Halide Exchange Mediated by a Cu <sup>I</sup> /Cu <sup>III</sup> Catalytic Cycle. Journal of the American Chemical Society, 2011, 133, 19386-19392.   | 13.7             | 232        |
| 239 | Editorial [Hot Topic: Electron Delocalization in Organic Chemistry (Guest Editors: Dr. Eduard Matito) Tj ETQq1 1 0  | .784314 r<br>1.6 | gBT/Overlo |
| 240 | Electron delocalization and aromaticity in low-lying excited states of archetypal organic compounds. Physical Chemistry Chemical Physics, 2011, 13, 20690.  | 2.8              | 116        |
| 241 | A multi-scale approach to spin crossover in Fe(ii) compounds. Physical Chemistry Chemical Physics, 2011, 13, 10449.   | 2.8              | 19         |
| 242 | Aromaticity and electronic delocalization in all-metal clusters with single, double, and triple aromatic character. Theoretical Chemistry Accounts, 2011, 128, 419-431.   | 1.4              | 57         |
| 243 | Measuring electron sharing between atoms in first-principle simulations. Theoretical Chemistry Accounts, 2011, 130, 27-36.  | 1.4              | 6          |
| 244 | Theoretical studies on aromaticity of selected hydroxypyrones. Part 3#. Chelatoaromaticity phenomenon in metalcomplexes of hydroxypyrones. Journal of Physical Organic Chemistry, 2011, 24, 499-506.                                | 1.9              | 16         |
| 245 | Performance of 3Dâ€spaceâ€based atomsâ€inâ€molecules methods for electronic delocalization aromaticity indices. Journal of Computational Chemistry, 2011, 32, 386-395.  | 3.3              | 36         |
| 246 | Inter―and intramolecular dispersion interactions. Journal of Computational Chemistry, 2011, 32, 1117-1127.  | 3.3              | 34         |
| 247 | A dissected ring current model for assessing magnetic aromaticity: A general approach for both organic and inorganic rings. Journal of Computational Chemistry, 2011, 32, 2422-2431.  | 3.3              | 61         |
| 248 | Intramolecular [2+2+2] Cycloaddition Reactions of Yneâ€eneâ€yne and Yneâ€yneâ€ene Enediynes Catalysed by Rh <sup>I</sup> : Experimental and Theoretical Mechanistic Studies. Chemistry - A European Journal, 2011, 17, 14493-14507. | 3.3              | 32         |
| 249 | The Chemical Reactivity of Fullerenes and Endohedral Fullerenes: A Theoretical Perspective. Carbon Materials, 2011, , 57-78.  | 1.2              | 2          |
| 250 | An account on multicenter bonding and its relationship with aromaticity. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C85-C85.   | 0.3              | 0          |
| 251 | 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.  | 2.8              | 38         |
| 252 | On the Mechanism of Action of Fullerene Derivatives in Superoxide Dismutation. Chemistry - A European Journal, 2010, 16, 3207-3214.   | 3.3              | 49         |

| #   | Article   | IF          | CITATIONS |
|-----|---|-------------|-----------|
| 253 | Reactivity and Regioselectivity of Noble Gas Endohedral Fullerenes Ng@C60 and Ng2@C60 (Ng=He-Xe). Chemistry - A European Journal, 2010, 16, 3878-3878.  | 3.3         | 6         |
| 254 | Spin-state splittings of iron(II) complexes with trispyrazolyl ligands. Polyhedron, 2010, 29, 84-93.  | 2.2         | 41        |
| 255 | A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity. Symmetry, 2010, 2, 1156-1179.   | 2.2         | 115       |
| 256 | 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. | <b>5.</b> 3 | 84        |
| 257 | Computational methods to predict the reactivity of nanoparticles through structure–property relationships. Expert Opinion on Drug Delivery, 2010, 7, 295-305.   | 5.0         | 64        |
| 258 | Mechanism of the Aminolysis of Fischer Alkoxy and Thiocarbene Complexes: A DFT Study. Journal of Organic Chemistry, 2010, 75, 5821-5836.  | 3.2         | 19        |
| 259 | Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2010, 6, 2736-2742.  | 5.3         | 115       |
| 260 | Density Functional Study of the [2+2+2] Cyclotrimerization of Acetylene Catalyzed by Wilkinson's Catalyst, RhCl(PPh <sub>3</sub> ) <sub>3</sub> . Organometallics, 2010, 29, 562-569.   | 2.3         | 68        |
| 261 | Density Functional Calculations of E2 and S <sub>N</sub> 2 Reactions: Effects of the Choice of Method, Algorithm, and Numerical Accuracy. Journal of Chemical Theory and Computation, 2010, 6, 3145-3152.                             | 5.3         | 33        |
| 262 | Influence of Confinement on Hydrogen Bond Energy. The Case of the FH···NCH Dimer. Journal of Physical Chemistry A, 2010, 114, 10253-10260.  | 2.5         | 31        |
| 263 | Facile Câ^'H Bond Cleavage via a Proton-Coupled Electron Transfer Involving a<br>Câ^'HÂ-Â-Â-Cu <sup>II</sup> Interaction. Journal of the American Chemical Society, 2010, 132, 12299-12306.   | 13.7        | 131       |
| 264 | Reaction Mechanisms for Graphene and Carbon Nanotube Fluorination. Journal of Physical Chemistry C, 2010, 114, 3340-3345.   | 3.1         | 56        |
| 265 | 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.  | 2.5         | 38        |
| 266 | Spin-State-Corrected Gaussian-Type Orbital Basis Sets. Journal of Physical Chemistry A, 2010, 114, 7191-7197.   | 2.5         | 47        |
| 267 | 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.   | <b>5.</b> 3 | 81        |
| 268 | Molecular mechanism of acid-triggered aryl–halide reductive elimination in well-defined aryl–Culll–halide species. Dalton Transactions, 2010, 39, 10458.  | 3.3         | 41        |
| 269 | Ene reactions between two alkynes? Doors open to thermally induced cycloisomerization of macrocyclic triynes and enediynes. Chemical Communications, 2010, 46, 2944.  | 4.1         | 23        |
| 270 | A new all-round density functional based on spin states and S[sub N]2 barriers. Journal of Chemical Physics, 2009, 131, 094103.   | 3.0         | 113       |

| #   | Article  | IF   | Citations |
|-----|--|------|-----------|
| 271 | Rhodium(I)â€Catalysed Intramolecular [2+2+2] Cyclotrimerisations of 15â€, 20†and 25â€Membered Azamacrocycles: Experimental and Theoretical Mechanistic Studies. Chemistry - A European Journal, 2009, 15, 5289-5300.                             | 3.3  | 49        |
| 272 | Reactivity and Regioselectivity of Noble Gas Endohedral Fullerenes Ng@C <sub>60</sub> and Ng <sub>2</sub> @C <sub>60</sub> (Ng=He–Xe). Chemistry - A European Journal, 2009, 15, 13111-13123.  | 3.3  | 45        |
| 273 | Dötz Benzannulation Reactions: Heteroatom and Substituent Effects in Chromium Fischer Carbene<br>Complexes. Chemistry - A European Journal, 2009, 15, 12503-12520.   | 3.3  | 21        |
| 274 | Homolytic versus Heterolytic Dissociation of Alkalimetal Halides: The Effect of Microsolvation. ChemPhysChem, 2009, 10, 2955-2965.   | 2.1  | 14        |
| 275 | 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.   | 2.0  | 15        |
| 276 | On the Regioselective Intramolecular Nucleophilic Addition of Thiols to C <sub>60</sub> . European Journal of Organic Chemistry, 2009, 2009, 6231-6238.  | 2.4  | 16        |
| 277 | Modeling the structureâ€property relationships of nanoneedles: A journey toward nanomedicine.<br>Journal of Computational Chemistry, 2009, 30, 275-284.  | 3.3  | 76        |
| 278 | Tuning aromaticity in trigonal alkaline earth metal clusters and their alkali metal salts. Journal of Computational Chemistry, 2009, 30, 2764-2776.  | 3.3  | 43        |
| 279 | Theoretical study of the hydroxylation of phenolates by the Cu2O2(N,N′-dimethylethylenediamine)2 2+ complex. Journal of Biological Inorganic Chemistry, 2009, 14, 229-242.   | 2.6  | 17        |
| 280 | Theoretical study of the hydroxylation of phenols mediated by an end-on bound superoxo–copper(II) complex. Journal of Biological Inorganic Chemistry, 2009, 14, 273-285.   | 2.6  | 12        |
| 281 | Excess charge delocalization in organic and biological molecules: some theoretical notions. Theoretical Chemistry Accounts, 2009, 123, 29-40.  | 1.4  | 9         |
| 282 | 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.                         | 18.8 | 141       |
| 283 | Dielsâ^'Alder Reaction between Cyclopentadiene and C <sub>60</sub> : 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, 9721-9726. | 2.5  | 63        |
| 284 | The Dielsâ^'Alder Reaction on Endohedral Y <sub>3</sub> N@C <sub>78</sub> : The Importance of the Fullerene Strain Energy. Journal of the American Chemical Society, 2009, 131, 129-139.   | 13.7 | 76        |
| 285 | 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, 1308-1317.   | 2.5  | 19        |
| 286 | Interplay between Intramolecular Resonance-Assisted Hydrogen Bonding and Local Aromaticity. II. 1,3-Dihydroxyaryl-2-aldehydes. Journal of Organic Chemistry, 2009, 74, 2059-2066.  | 3.2  | 68        |
| 287 | H-Bond-Assisted Regioselective ( <i>cis-1</i> ) Intramolecular Nucleophilic Addition of the Hydroxyl Group to [60]Fullerene. Journal of Organic Chemistry, 2009, 74, 1480-1487.  | 3.2  | 37        |
| 288 | Competitive Retro-Cycloaddition Reaction in Fullerene Dimers Connected through Pyrrolidinopyrazolino Rings. Journal of Organic Chemistry, 2009, 74, 8174-8180.   | 3.2  | 25        |

| #   | Article  | IF       | Citations                |
|-----|--|----------|--------------------------|
| 289 | Regioselective Intramolecular Nucleophilic Addition of Alcohols to C <sub>60</sub> : One-Step Formation of a <i>ci&gt;&lt; i&gt;-1 Bicyclic-Fused Fullerene. Journal of Organic Chemistry, 2009, 74, 6253-6259.</i>                        | 3.2      | 33                       |
| 290 | Local Aromaticity of Pristine and Fluorinated Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2009, 9, 6078-6083.   | 0.9      | 8                        |
| 291 | Aromaticity and Chemical Reactivity. , 2009, , .   |          | 5                        |
| 292 | On the Mechanism of the Thermal Retrocycloaddition of Pyrrolidinofullerenes (Retroâ€Prato) Tj ETQq0 0 0 rgBT /   | Oyerlock | 10 <sub>.56</sub> 50 622 |
| 293 | The hardness kernel as the basis for global and local reactivity indices. Journal of Computational Chemistry, 2008, 29, 1064-1072.   | 3.3      | 34                       |
| 294 | On the performance of some aromaticity indices: A critical assessment using a test set. Journal of Computational Chemistry, 2008, 29, 1543-1554.   | 3.3      | 261                      |
| 295 | Mechanistic theoretical insight of Ru(II) catalysts with a meridional–facial bpea fashion competition.<br>Chemical Physics Letters, 2008, 458, 200-204.  | 2.6      | 10                       |
| 296 | Coordination of bis(tricarbonylchromium) complexes to small polycyclic aromatic hydrocarbons: Structure, relative stabilities, and bonding. Chemical Physics Letters, 2008, 465, 181-189.  | 2.6      | 7                        |
| 297 | Nanosized trigonal prismatic and antiprismatic Cull coordination cages based on tricarboxylate linkers. Dalton Transactions, 2008, , 1679.   | 3.3      | 15                       |
| 298 | E2 and S <sub>N</sub> 2 Reactions of X <sup><math>\hat{a}^{\circ}</math></sup> + CH <sub>3</sub> CH <sub>2</sub> X (X = F, Cl); an <i>ab Initio</i> and DFT Benchmark Study. Journal of Chemical Theory and Computation, 2008, 4, 929-940. | 5.3      | 86                       |
| 299 | Analysis of Hückel's [4 <i>n</i> + 2] Rule through Electronic Delocalization Measures. Journal of Physical Chemistry A, 2008, 112, 13231-13238.  | 2.5      | 38                       |
| 300 | Complete Mechanism of $lf^*$ Intramolecular Aromatic Hydroxylation through O <sub>2</sub> Activation by a Macrocyclic Dicopper(I) Complex. Journal of the American Chemical Society, 2008, 130, 17710-17717.                               | 13.7     | 62                       |
| 301 | Importance of the Basis Set for the Spin-State Energetics of Iron Complexes. Journal of Physical Chemistry A, 2008, 112, 6384-6391.  | 2.5      | 131                      |
| 302 | New Ruthenium(II) Complexes with Enantiomerically Pure Bis- and Tris(pinene)-Fused Tridentate Ligands. Synthesis, Characterization and Stereoisomeric Analysis. Inorganic Chemistry, 2008, 47, 8016-8024.                                  | 4.0      | 16                       |
| 303 | Coordination and Haptotropic Migration of Cr(CO) <sub>3</sub> in Polycyclic Aromatic Hydrocarbons:  The Effect of the Size and the Curvature of the Substrate. Journal of Physical Chemistry A, 2008, 112, 1202-1213.                      | 2.5      | 33                       |
| 304 | Intramolecular Haptotropic Rearrangements of the Tricarbonylchromium Complex in Small Polycyclic Aromatic Hydrocarbons. Organometallics, 2008, 27, 5230-5240.  | 2.3      | 31                       |
| 305 | Chemical Reactivity of D3h C78 (Metallo)Fullerene: Regioselectivity Changes Induced by Sc3N Encapsulation. Journal of the American Chemical Society, 2008, 130, 6206-6214.   | 13.7     | <b>7</b> 5               |
| 306 | Chapter 3 The breakdown of the maximum hardness and minimum polarizability principles for nontotally symmetric vibrations. Theoretical and Computational Chemistry, 2007, , 31-45.   | 0.4      | 2                        |

| #   | Article   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 307 | Chapter 10 Electronic structure and reactivity of aromatic metal clusters. Theoretical and Computational Chemistry, 2007, 19, 203-218.  | 0.4 | O         |
| 308 | Mechanistic Insights into the Chemistry of Ru(II) Complexes Containing Cl and DMSO Ligands. Inorganic Chemistry, 2007, 46, 10707-10716.   | 4.0 | 53        |
| 309 | New Solids Based on B <sub>12</sub> N <sub>12</sub> Fullerenes. Journal of Physical Chemistry C, 2007, 111, 13354-13360.  | 3.1 | 72        |
| 310 | Electron sharing indexes at the correlated level. Application to aromaticity calculations. Faraday Discussions, 2007, 135, 325-345.   | 3.2 | 203       |
| 311 | Highly polar bonds and the meaning of covalency and ionicityâ€"structure and bonding of alkali metal hydride oligomers. Faraday Discussions, 2007, 135, 451-468.                          | 3.2 | 19        |
| 312 | Theoretical Study of the Reaction Mechanisms Involved in the Thermal Intramolecular Reactions of 1,6-Fullerenynes. Journal of Physical Chemistry A, 2007, 111, 5253-5258.                 | 2.5 | 12        |
| 313 | Aromaticity of Distorted Benzene Rings:  Exploring the Validity of Different Indicators of Aromaticity. Journal of Physical Chemistry A, 2007, 111, 4513-4521.                            | 2.5 | 102       |
| 314 | Didehydrophenanthrenes:  Structure, Singletâ^'Triplet Splitting, and Aromaticity. Journal of Physical Chemistry A, 2007, 111, 5063-5070.  | 2.5 | 39        |
| 315 | Table Salt and Other Alkali Metal Chloride Oligomers:  Structure, Stability, and Bonding. Inorganic Chemistry, 2007, 46, 5411-5418.   | 4.0 | 17        |
| 316 | Fast O2Binding at Dicopper Complexes Containing Schiff-Base Dinucleating Ligands. Inorganic Chemistry, 2007, 46, 4997-5012.   | 4.0 | 43        |
| 317 | Properties of Aromaticity Indices Based on the One-Electron Density Matrix. Journal of Physical Chemistry A, 2007, 111, 6521-6525.  | 2.5 | 118       |
| 318 | Polycyclic Benzenoids:Â Why Kinked is More Stable than Straight. Journal of Organic Chemistry, 2007, 72, 1134-1142.   | 3.2 | 197       |
| 319 | On the quality of the hardness kernel and the Fukui function to evaluate the global hardness. Journal of Computational Chemistry, 2007, 28, 574-583.                                      | 3.3 | 48        |
| 320 | Covalentversus ionic bonding in alkalimetal fluoride oligomers. Journal of Computational Chemistry, 2007, 28, 238-250.  | 3.3 | 18        |
| 321 | Energy landscapes of nucleophilic substitution reactions: A comparison of density functional theory and coupled cluster methods. Journal of Computational Chemistry, 2007, 28, 1551-1560. | 3.3 | 89        |
| 322 | Electron delocalization and aromaticity measures within the H $\tilde{A}^{1}\!\!/\!\!4$ ckel molecular orbital method. Computational and Theoretical Chemistry, 2007, 811, 3-11.          | 1.5 | 46        |
| 323 | Aromaticity changes along the reaction coordinate connecting the cyclobutadiene dimer to cubane and the benzene dimer to hexaprismane. Structural Chemistry, 2007, 18, 773-783.           | 2.0 | 18        |
| 324 | The proton transfer reaction in malonaldehyde derivatives: Substituent effects and quasi-aromaticity of the proton bridge. Chemical Physics, 2007, 342, 43-54.                            | 1,9 | 43        |

| #   | Article   | IF              | CITATIONS   |
|-----|---|-----------------|-------------|
| 325 | 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.                    | 3.2             | 57          |
| 326 | Copper(II) Hexaaza Macrocyclic Binuclear Complexes Obtained from the Reaction of Their Copper(I) Derivates and Molecular Dioxygen. Inorganic Chemistry, 2006, 45, 3569-3581.  | 4.0             | 61          |
| 327 | Pseudo-Jahnâ^'Teller Effect as the Origin of the Exalted Frequency of the b2u Kekulé Mode in the 1B2u Excited State of Benzene. Journal of Physical Chemistry A, 2006, 110, 11219-11222.                                    | 2.5             | 23          |
| 328 | 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.                  | 3.3             | 70          |
| 329 | Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. Journal of Physical Chemistry A, 2006, 110, 12249-12258.  | 2.5             | 52          |
| 330 | 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, 5108-5113.                                    | 2.5             | 76          |
| 331 | Interplay between Intramolecular Resonance-Assisted Hydrogen Bonding and Aromaticity in o-Hydroxyaryl Aldehydes. Journal of Organic Chemistry, 2006, 71, 5241-5248.   | 3.2             | 110         |
| 332 | 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.                             | 2.3             | 19          |
| 333 | 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, 8901-8911. | 2.5             | 8           |
| 334 | New Ru Complexes Containing the N-Tridentate bpea and Phosphine Ligands:Â Consequences of Meridional vs Facial Geometry. Inorganic Chemistry, 2006, 45, 10520-10529.  | 4.0             | 41          |
| 335 | Covalency in Highly Polar Bonds. Structure and Bonding of Methylalkalimetal Oligomers (CH3M)n (M) Tj ETQq1 1  | 0.784314<br>5.3 | ŀrgBT /Over |
| 336 | Redox-Controlled Molecular Flipper Based on a Chiral Cu Complex. Inorganic Chemistry, 2006, 45, 9643-9645.  | 4.0             | 10          |
| 337 | 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.  | 2.6             | 39          |
| 338 | Electron localization function at the correlated level. Journal of Chemical Physics, 2006, 125, 024301.   | 3.0             | 135         |
| 339 | Intramolecular Ene Reaction of 1,6-Fullerenynes:  A New Synthesis of Allenes. Organic Letters, 2006, 8, 5959-5962.  | 4.6             | 33          |
| 340 | O2Chemistry of Dicopper Complexes with Alkyltriamine Ligands. Comparing Synergistic Effects on O2Binding. Inorganic Chemistry, 2006, 45, 5239-5241.   | 4.0             | 26          |
| 341 | Molecular Structure and Bonding of Copper Cluster Monocarbonyls CunCO (n= 1â^9). Journal of Physical Chemistry B, 2006, 110, 6526-6536.   | 2.6             | 97          |
| 342 | Are nucleus-independent (NICS) and 1H NMR chemical shifts good indicators of aromaticity in π-stacked polyfluorenes?. Chemical Physics Letters, 2006, 428, 191-195.   | 2.6             | 33          |

| #   | Article   | IF   | Citations |
|-----|---|------|-----------|
| 343 | Nucleus-independent chemical shift (NICS) profiles in a series of monocyclic planar inorganic compounds. Journal of Organometallic Chemistry, 2006, 691, 4359-4366.   | 1.8  | 155       |
| 344 | 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.   | 2.5  | 28        |
| 345 | Structure and bonding of methyl alkali metal molecules. Journal of Molecular Modeling, 2006, 12, 563-568.   | 1.8  | 11        |
| 346 | Theoretical Evaluation of Electron Delocalization in Aromatic Molecules by Means of Atoms in Molecules (AIM) and Electron Localization Functional (ELF) Topological Approaches. ChemInform, 2006, 37, no.   | 0.0  | 0         |
| 347 | Atropisomeric Discrimination in New Rull Complexes Containing the C2-Symmetric Didentate Chiral Phenyl-1,2-bisoxazolinic Ligand. Chemistry - A European Journal, 2006, 12, 2798-2807.   | 3.3  | 30        |
| 348 | Hydrogen–Hydrogen Bonding in Planar Biphenyl, Predicted by Atoms-In-Molecules Theory, Does Not Exist. Chemistry - A European Journal, 2006, 12, 2889-2895.  | 3.3  | 314       |
| 349 | 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.  | 3.3  | 216       |
| 350 | Thermal [2+2] Intramolecular Cycloadditions of Fuller-1,6-enynes. Angewandte Chemie - International Edition, 2006, 45, 1439-1442.   | 13.8 | 53        |
| 351 | Regiospecific CH Bond Activation: Reversible H/D Exchange Promoted by Cul Complexes with Triazamacrocyclic Ligands. Angewandte Chemie - International Edition, 2006, 45, 2941-2944.  | 13.8 | 42        |
| 352 | Electron Fluctuation in Pericyclic and Pseudopericyclic Reactions. ChemPhysChem, 2006, 7, 111-113.  | 2.1  | 45        |
| 353 | Chemical bonding in transition metal carbene complexes. Journal of Organometallic Chemistry, 2005, 690, 6178-6204.  | 1.8  | 206       |
| 354 | 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        |
| 355 | Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1â^9). Journal of Organic Chemistry, 2005, 70, 2509-2521.  | 3.2  | 195       |
| 356 | Oxidative addition of the ethane Ci£¿C bond to Pd. Anab initiobenchmark and DFT validation study. Journal of Computational Chemistry, 2005, 26, 1006-1020.  | 3.3  | 69        |
| 357 | Ab initio and DFT benchmark study for nucleophilic substitution at carbon (SN2@C) and silicon (SN2@Si). Journal of Computational Chemistry, 2005, 26, 1497-1504.  | 3.3  | 133       |
| 358 | Aromaticity Analysis of Lithium Cation/ π Complexes of Aromatic Systems. ChemPhysChem, 2005, 6, 2552-2561.  | 2.1  | 46        |
| 359 | Regioselective Intramolecular Pauson-Khand Reactions of C60: An Electrochemical Study and Theoretical Underpinning. Chemistry - A European Journal, 2005, 11, 2716-2729.  | 3.3  | 58        |
| 360 | Fine-Tuning the Electronic Properties of Highly Stable Organometallic Culll Complexes Containing Monoanionic Macrocyclic Ligands. Chemistry - A European Journal, 2005, 11, 5146-5156.  | 3.3  | 106       |

| #   | Article   | IF   | Citations |
|-----|---|------|-----------|
| 361 | The Breakdown of the Minimum Polarizability Principle in Vibrational Motions as an Indicator of the Most Aromatic Center. Chemistry - A European Journal, 2005, 11, 6024-6031.  | 3.3  | 15        |
| 362 | Basis set effects on the energy and hardness profiles of the hydrogen fluoride dimer. Journal of Chemical Sciences, 2005, 117, 549-554.   | 1.5  | 4         |
| 363 | Ab initio and DFT modeling of stereoselective deamination of aziridines by nitrosyl chloride.<br>International Journal of Quantum Chemistry, 2005, 102, 139-146.  | 2.0  | 9         |
| 364 | 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.   | 1.9  | 147       |
| 365 | Calculation of Franck–Condon factors including anharmonicity: Simulation of the C2H4+XÌfB3u2ↀ2H4XÌfAg1 band in the photoelectron spectrum of ethylene. Journal of Chemical Physics, 2005, 122, 184104.                      | 3.0  | 25        |
| 366 | The aromatic fluctuation index (FLU): A new aromaticity index based on electron delocalization. Journal of Chemical Physics, 2005, 122, 014109.   | 3.0  | 396       |
| 367 | 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.                       | 1.5  | 31        |
| 368 | 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.       | 47.7 | 661       |
| 369 | Local Aromaticity of the Lowest-Lying Singlet States of $[n]$ Acenes $(n = 6a^2)$ . Journal of Physical Chemistry A, 2005, 109, 10629-10632.  | 2.5  | 68        |
| 370 | 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.   | 1.7  | 32        |
| 371 | Generalizing the Breakdown of the Maximum Hardness and Minimum Polarizabilities Principles for Nontotally Symmetric Vibrations to Non-ï€-Conjugated Organic Molecules. Journal of Physical Chemistry A, 2005, 109, 615-621. | 2.5  | 26        |
| 372 | 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.                                       | 2.6  | 17        |
| 373 | Comparison of the AIM Delocalization Index and the Mayer and Fuzzy Atom Bond Orders. Journal of Physical Chemistry A, 2005, 109, 9904-9910.   | 2.5  | 169       |
| 374 | Diastereoselective Synthesis of Fulleropyrrolidines from Suitably Functionalized Chiral Cyclobutanes. Journal of Organic Chemistry, 2005, 70, 6929-6932.  | 3.2  | 22        |
| 375 | 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, 3256-3262.    | 3.2  | 36        |
| 376 | The hardness profile as a tool to detect spurious stationary points in the potential energy surface. Journal of Chemical Physics, 2004, 120, 10914-10924.   | 3.0  | 32        |
| 377 | Basis set and electron correlation effects on initial convergence for vibrational nonlinear optical properties of conjugated organic molecules. Journal of Chemical Physics, 2004, 120, 6346-6355.                          | 3.0  | 60        |
| 378 | Relation between the Substituent Effect and Aromaticity. Journal of Organic Chemistry, 2004, 69, 6634-6640.   | 3.2  | 177       |

| #   | Article   | IF                  | CITATIONS                 |
|-----|---|---------------------|---------------------------|
| 379 | Analysis of electronic delocalization in buckminsterfullerene (C60). International Journal of Quantum Chemistry, 2004, 98, 361-366.   | 2.0                 | 23                        |
| 380 | 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, 439-446.  | 3.3                 | 13                        |
| 381 | Discrepancy Between Common Local Aromaticity Measures in a Series of Carbazole Derivatives.<br>ChemInform, 2004, 35, no.  | 0.0                 | 0                         |
| 382 | Ground and Low-Lying States of Cu2+—H2O. A Difficult Case for Density Functional Methods<br>ChemInform, 2004, 35, no.   | 0.0                 | 0                         |
| 383 | 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, 9982-9992.   | 3.0                 | 73                        |
| 384 | 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.   | 3.2                 | 113                       |
| 385 | Quantum Chemical Study of the Reactivity of C60HR and C60(CHR) Derivatives. Journal of Organic Chemistry, 2004, 69, 2374-2380.  | 3.2                 | 9                         |
| 386 | 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.  | 2.5                 | 85                        |
| 387 | Discrepancy between common local aromaticity measures in a series of carbazole derivatives. Physical Chemistry Chemical Physics, 2004, 6, 314-318.  | 2.8                 | 106                       |
| 388 | Stereodiscrimination in Phosphanylthiolato Nickel(II) Complexes. European Journal of Inorganic Chemistry, 2003, 2003, 4147-4151.  | 2.0                 | 14                        |
| 389 | An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes<br>ChemInform, 2003, 34, no.   | 0.0                 | 0                         |
| 390 | 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.                                      | 3.3                 | 396                       |
| 391 | An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes.<br>Chemistry - A European Journal, 2003, 9, 1113-1122.  | 3.3                 | 125                       |
| 392 | Electron pairing analysis of the Fischer-type chromium–carbene complexes (CO)5Crĩ…C(X)R (X=H, OH,) Tj ETC   | 2q <u>0,</u> 9 0 rg | BT <sub>18</sub> Overlock |
| 393 | 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.   | 2.6                 | 74                        |
| 394 | Evaluation of the Analogy between Exceptions to the Generalized Maximum Hardness Principle for Non-Totally-Symmetric Vibrations and the Pseudo-Jahnâ^*Teller Effect. Journal of Physical Chemistry A, 2003, 107, 7337-7339. | 2.5                 | 18                        |
| 395 | Dinuclear Copper(I) Complexes with Hexaaza Macrocyclic Dinucleating Ligands:  Structure and Dynamic Properties. Inorganic Chemistry, 2003, 42, 4456-4468.   | 4.0                 | 21                        |
| 396 | 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.                           | 3.0                 | 105                       |

| #   | Article  | IF   | CITATIONS |
|-----|--|------|-----------|
| 397 | Relations among several nuclear and electronic density functional reactivity indexes. Journal of Chemical Physics, 2003, 119, 9393-9400.   | 3.0  | 22        |
| 398 | Are the maximum hardness and minimum polarizability principles always obeyed in nontotally symmetric vibrations?. Journal of Chemical Physics, 2002, 117, 10561-10570.   | 3.0  | 77        |
| 399 | BIELECTRONIC DENSITIES: ANALYSIS AND APPLICATIONS IN MOLECULAR STRUCTURE AND CHEMICAL REACTIVITY., 2002, , 831-870.  |      | 2         |
| 400 | Isolation and Characterization of Four Isomers of a C60Bisadduct with a TTF Derivative. Study of Their Radical Ions. Journal of Organic Chemistry, 2002, 67, 566-575.  | 3.2  | 22        |
| 401 | Molecular Structure and Bond Characterization of the Fischer-Type Chromiumâ^'Carbene Complexes (CO)5CrC(X)R (X = H, OH, OCH3, NH2, NHCH3 and R = H, CH3, CHCH2, Ph, Câ $^{\circ}$ CH). Organometallics, 2002, 21, 4182-4191.                 | 2.3  | 80        |
| 402 | Global Hardness Evaluation Using Simplified Models for the Hardness Kernel. Journal of Physical Chemistry A, 2002, 106, 4632-4638.   | 2.5  | 29        |
| 403 | Initial convergence of the perturbation series expansion for vibrational nonlinear optical properties. Journal of Chemical Physics, 2002, 116, 5363-5373.  | 3.0  | 43        |
| 404 | Analysis of the effect of changing the aO 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. | 2.8  | 51        |
| 405 | Electron localization and delocalization in open-shell molecules. Journal of Computational Chemistry, 2002, 23, 1347-1356.   | 3.3  | 34        |
| 406 | The calculation of electron localization and delocalization indices at the Hartree-Fock, density functional and post-Hartree-Fock levels of theory. Theoretical Chemistry Accounts, 2002, 107, 362-371.                                      | 1.4  | 187       |
| 407 | Electron-pairing analysis from localization and delocalization indices in the framework of the atoms-in-molecules theory. Theoretical Chemistry Accounts, 2002, 108, 214-224.  | 1.4  | 175       |
| 408 | PRISTINE AND SILICON-SUBSTITUTED SMALL-CARBON-CLUSTERS AND FULLERENES: ELECTRONIC STRUCTURE AND REACTIVITY., 2002, , 1367-1420.  |      | 2         |
| 409 | A Theoretical Study of Steric and Electronic Effects in the Rhodium-Catalyzed Carbonylation Reactions. Journal of the American Chemical Society, 2001, 123, 12294-12302.   | 13.7 | 63        |
| 410 | On the Validity of the Maximum Hardness and Minimum Polarizability Principles for Nontotally Symmetric Vibrations. Journal of the American Chemical Society, 2001, 123, 7951-7952.   | 13.7 | 112       |
| 411 | Mechanism of the Addition Reaction of Alkyl Azides to [60]Fullerene and the Subsequent N2Extrusion to Form Monoimino-[60]fullerenes. Journal of Organic Chemistry, 2001, 66, 433-442.  | 3.2  | 91        |
| 412 | 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.       | 2.3  | 15        |
| 413 | New Insights in Chemical Reactivity by Means of Electron Pairing Analysis. Journal of Physical Chemistry A, 2001, 105, 2052-2063.  | 2.5  | 34        |
| 414 | 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.  | 2.5  | 32        |

| #   | Article   | IF   | Citations |
|-----|---|------|-----------|
| 415 | Density functional theory study of the structures and stabilities of CuO and CuO3. International Journal of Quantum Chemistry, 2001, 81, 162-168.   | 2.0  | 11        |
| 416 | 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.   | 3.3  | 21        |
| 417 | Density functional theory study of the structures and stabilities of CuO and CuO3. International Journal of Quantum Chemistry, 2001, 81, 162-168.   | 2.0  | 0         |
| 418 | 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.                       | 3.3  | 11        |
| 419 | Substituent effects on the intramolecular proton transfer in the ground and lowest-lying singlet excited states of salicylaldimine. Chemical Physics, 2000, 260, 53-64.   | 1.9  | 22        |
| 420 | The [2+1] Cycloaddition of Singlet Oxycarbonylnitrenes to C 60. Journal of Molecular Modeling, 2000, 6, 205-212.  | 1.8  | 14        |
| 421 | Theoretical Studies of Some Transition-Metal-Mediated Reactions of Industrial and Synthetic Importance. Chemical Reviews, 2000, 100, 439-494.   | 47.7 | 371       |
| 422 | 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.                           | 3.3  | 0         |
| 423 | Theoretical Evaluation of Solvent Effects on the Conformational and Tautomeric Equilibria of 2-( $2\hat{a}\in^{\sim}$ -Hydroxyphenyl)benzimidazole and on Its Absorption and Fluorescence Spectra. Journal of Physical Chemistry A, 1999, 103, 4525-4532. | 2.5  | 79        |
| 424 | Weighing Different Mechanistic Proposals for the Dötz Reaction: A Density Functional Study. Journal of the American Chemical Society, 1999, 121, 1309-1316.   | 13.7 | 37        |
| 425 | Excited-State Intramolecular Proton Transfer and Rotamerism of 2-(2â€~-hydroxyvinyl)benzimidazole and 2-(2â€~-hydroxyphenyl)imidazole. Journal of Physical Chemistry A, 1999, 103, 4413-4420.   | 2.5  | 78        |
| 426 | 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.  | 2.3  | 55        |
| 427 | The Hammond Postulate and the Principle of Maximum Hardness in Some Intramolecular Rearrangement Reactions. Journal of Physical Chemistry A, 1999, 103, 8847-8852.  | 2.5  | 62        |
| 428 | Optimizing hybrid density functionals by means of quantum molecular similarity techniques. Advances in Molecular Similarity, $1999$ , , $187-203$ .   | 0.5  | 2         |
| 429 | Exploring the possibility of a bimolecular reaction channel for the F2SS/FSSF rearrangement process. Computational and Theoretical Chemistry, 1998, 455, 123-129.   | 1.5  | 5         |
| 430 | 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.  | 2.0  | 31        |
| 431 | 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.  | 1.9  | 24        |
| 432 | Low-lying electronic states and molecular structure of Fe2O2. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2877-2881.   | 1.7  | 9         |

| #   | Article  | IF   | Citations |
|-----|--|------|-----------|
| 433 | Density Functional Study on the Preactivation Scenario of the Dötz Reaction:  Carbon Monoxide Dissociation versus Alkyne Addition as the First Reaction Step. Organometallics, 1998, 17, 1492-1501.                                | 2.3  | 34        |
| 434 | Dielsâ^'Alder Cycloadditions of 1,3-Butadiene to Polycyclic Aromatic Hydrocarbons (PAH). Quantifying the Reactivity Likeness of Bowl-Shaped PAHs to C60. Journal of Organic Chemistry, 1998, 63, 7556-7558.                        | 3.2  | 24        |
| 435 | Theoretical Study on the Thermodynamics of the Elimination of Formic Acid in the Last Step of the Hydrogenation of CO2Catalyzed by Rhodium Complexes in the Gas Phase and Supercritical CO2. Organometallics, 1998, 17, 3164-3168. | 2.3  | 39        |
| 436 | Density Functional Study of the [2+2]- and [2+3]-Cycloaddition Mechanisms for the Osmium-Catalyzed Dihydroxylation of Olefins. Organometallics, 1997, 16, 13-19.   | 2.3  | 122       |
| 437 | 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.                                      | 2.3  | 10        |
| 438 | 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.           | 2.4  | 10        |
| 439 | Low-lying electronic states and molecular structure of FeO2 and FeO2â^'. Chemical Physics Letters, 1997, 274, 411-421.   | 2.6  | 26        |
| 440 | Theoretical Study on Acetaldehyde and Ethanol Elimination from the Hydrogenation of CH3(O)CCo(CO)3. Organometallics, 1996, 15, 2611-2618.  | 2.3  | 49        |
| 441 | Theoretical Study of the Regioselectivity of Successive 1,3-Butadiene Dielsâ^'Alder Cycloadditions to C60. Journal of the American Chemical Society, 1996, 118, 8920-8924.   | 13.7 | 37        |
| 442 | 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.             | 3.0  | 54        |
| 443 | 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.                                     | 1.5  | 27        |
| 444 | Analysis of the changes on the potential energy surface of Menshutkin reactions induced by external perturbations. Computational and Theoretical Chemistry, 1996, 371, 171-183.  | 1.5  | 26        |
| 445 | 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.                                 | 2.9  | 27        |
| 446 | Exploring chromium (VI) dioxodihalides chemistry: Is density functional theory the most suitable tool?. Journal of Chemical Physics, 1996, 104, 9499-9510.   | 3.0  | 28        |
| 447 | Theoretical Study of Dielsâ^'Alder Cycloadditions of Butadiene to C70. An Insight into the Chemical Reactivity of C70as Compared to C60. The Journal of Physical Chemistry, 1996, 100, 7449-7454.                                  | 2.9  | 64        |
| 448 | The use of ab initio quantum molecular selfâ€similarity measures to analyze electronic charge density distributions. International Journal of Quantum Chemistry, 1996, 58, 361-372.  | 2.0  | 25        |
| 449 | How similar are HF, MP2, and DFT charge distributions in the Cr(CO)6 complex?. Advances in Molecular Similarity, 1996, , 167-186.  | 0.5  | 2         |
| 450 | 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.  | 3.3  | 52        |

| #   | Article  | IF             | CITATIONS         |
|-----|--|----------------|-------------------|
| 451 | Molecular Size and Pyramidalization: Two Keys for Understanding the Reactivity of Fullerenes. The Journal of Physical Chemistry, 1995, 99, 10752-10758.  | 2.9            | 50                |
| 452 | Ab initio study of the HCO 3?/H2O exchange in the (NH3)3 ZnII(HCO 3?) complex. Theoretica Chimica Acta, 1995, 91, 333-351.   | 0.8            | 1                 |
| 453 | 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.                      | 0.9            | 5                 |
| 454 | Foundations and recent developments on molecular quantum similarity. Topics in Current Chemistry, 1995, , 31-62.   | 4.0            | 72                |
| 455 | An AM1 study of the reactivity of buckminsterfullerene (C60) in a Diels-Alder model reaction. Chemical Physics Letters, 1994, 231, 325-330.  | 2.6            | 49                |
| 456 | On the calculation of ab initioquantum molecular similarities for large systems: Fitting the electron density. Journal of Computational Chemistry, 1994, 15, 1113-1120.                            | 3.3            | 46                |
| 457 | 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.                                      | 0.9            | 8                 |
| 458 | 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.                     | 13.7           | 54                |
| 459 | Ab Initio Quantum Molecular Similarity Measures on Metal-Substituted Carbonic Anhydrase (MIICA, M) Tj ETQq1 I  | 0.78431<br>2.8 | 4 rgBT /Ove<br>25 |
| 460 | 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. | 13.7           | 70                |
| 461 | Valence-bond calculations on ZNO and HGO using integrals computed through the semiempiricalAM1 method. International Journal of Quantum Chemistry, 1992, 44, 887-895.                              | 2.0            | 2                 |
| 462 | Ab initio study of the effect of external perturbations in the dissociation of CH3Cl. Computational and Theoretical Chemistry, 1992, 255, 283-296.   | 1.5            | 8                 |
| 463 | Theoretical Study of the Catalyzed Hydration of CO2 by Carbonic Anhydrase: A Brief Overview, 1992,, 263-298.   |                | 2                 |
| 464 | Anion binding and pentacoordination in zinc(II) complexes. Inorganic Chemistry, 1991, 30, 2523-2527.   | 4.0            | 31                |
| 465 | Analysis of solvent effects on the Menshutkin reaction. Journal of the American Chemical Society, 1991, 113, 2873-2879.  | 13.7           | 123               |
| 466 | 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.                     | 2.0            | 7                 |
| 467 | Ab initiostudy of substituent effect on the addition of hydrogen fluoride to fluoroethylenes. Journal of Computational Chemistry, 1990, 11, 170-180.   | 3.3            | 13                |
| 468 | Aromaticity Analysis by Means of the Quantum Theory of Atoms in Molecules. , 0, , 399-423.   |                | 6                 |

## Miquel SolÃ

| #   | Article   | IF          | CITATIONS |
|-----|---|-------------|-----------|
| 469 | One Century of Physical Organic Chemistry: The Menshutkin Reaction. Progress in Physical Organic Chemistry, 0, , 1-182.   | 1.2         | 47        |
| 470 | A Rh(I) $\hat{a}\in \mathbb{C}$ atalyzed Cascade Cyclization of 1,5 $\hat{a}\in \mathbb{B}$ isallenes and Alkynes for the Formation of cis $\hat{a}\in \mathbb{A}$ ,4 $\hat{a}\in \mathbb{A}$ rylvinyl Pyrrolidines and Cyclopentanes. Advanced Synthesis and Catalysis, 0, , . | <b>4.</b> 3 | 3         |
| 471 | Aromaticity and Extrusion of Benzenoids Linked to [ <i>&gt;o</i> OSAN] <sup>â^²</sup> : Clar Has the Answer. Angewandte Chemie, 0, , .  | 2.0         | 3         |