Ricardo A Mosquera

List of Publications by Year
in descending order

139	2,569	218381	288905
papers	citations	26 h-index	40 g-index

141	141	141	2008
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	First Characterization of the Formation of Anthocyaninâ€“Ge and Anthocyaninâ€“B Complexes through UVâ€“Vis Spectroscopy and Density Functional Theory Quantum Chemical Calculations. Journal of Agricultural and Food Chemistry, 2021, 69, 1272-1282.	2.4	22
2	Do oneâ€step mechanisms always involve simultaneous evolution of electron density? QTAIM/IQA analysis of the Curtius rearrangement. International Journal of Quantum Chemistry, 2020, 120, e26170.	1.0	3
3	Chiroptical Symmetry Analysis of Trianglimines: A Case Study. Symmetry, 2019, 11, 1245.	1.1	3
4	Chiroptical Symmetry Analysis: Exciton Chirality-Based Formulae to Understand the Chiroptical Responses of Cn and Dn Symmetric Systems. Molecules, 2019, 24, 141.	1.7	5
5	Complexation of common metal cations by cyanins: Binding affinity and molecular structure. International Journal of Quantum Chemistry, 2019, 119, e25834.	1.0	11
6	Driving Forces in the Sharpless Epoxidation Reaction: A Coupled AIMD/QTAIM Study. Inorganic Chemistry, 2017, 56, 2124-2134.	1.9	9
7	On the effects of the basis set superposition error on the change of QTAIM charges in adduct formation. Application to complexes between morphine and cocaine and their main metabolites. RSC Advances, 2016, 6, 110642-110655.	1.7	2
8	How Electronic Excitation Can be Used to Inhibit Some Mechanisms Associated to Substituent Effects. ChemPhysChem, 2016, 17, 2666-2671.	1.0	9
9	Roots of Acetate-Vanadium Linkage Isomerism: A QTAIM Study. Inorganic Chemistry, 2016, 55, 3653-3662.	1.9	9
10	Revisiting Lewis dot structure weightings: a pair density perspective. Physical Chemistry Chemical Physics, 2015, 17, 7424-7434.	1.3	5
11	Revisiting the carbonyl n â†' Ï€* electronic excitation through topological eyes: expanding, enriching and enhancing the chemical language using electron number distribution functions and domain averaged Fermi holes. Physical Chemistry Chemical Physics, 2015, 17, 26059-26071.	1.3	3
12	Excluding hyperconjugation from the Z conformational preference and investigating its origin: formic acid and beyond. Physical Chemistry Chemical Physics, 2015, 17, 26946-26954.	1.3	5
13	Exploring the versatility of the gCH topological electronegativity estimator. Computational and Theoretical Chemistry, 2015, 1053, 85-89.	1.1	2
14	When valence bond wave functions are analyzed through QTAIM: Conceptual incompatibilities in H2. Chemical Physics Letters, 2015, 618, 83-88.	1.2	4
15	Computational Studies on Conformation, Electron Density Distributions, and Antioxidant Properties of Anthocyanidins. Methods in Molecular Biology, 2015, 1208, 257-276.	0.4	4
16	Charge distribution in Mn(salen) complexes. International Journal of Quantum Chemistry, 2014, 114, 525-533.	1.0	12
17	On the structure of Zn(II) and Cu(II) cyanin complexes in aqueous solution. Structural Chemistry, 2014, 25, 1647-1657.	1.0	2
18	Effects of Axial Coordination on Immobilized Mn(salen) Catalysts. Journal of Physical Chemistry A, 2014, 118, 10788-10796.	1.1	10

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19	Beyond the molecular orbital conception of electronically excited states through the quantum theory of atoms in molecules. Physical Chemistry Chemical Physics, 2014, 16, 9249-9258.	1.3	36
20	Principal component analysis of Mn(salen) catalysts. Physical Chemistry Chemical Physics, 2014, 16, 25364-25376.	1.3	13
21	Understanding the electron density reorganization upon stacking vs. H-bonding interaction in methyl gallateâ€“caffeine complexes. RSC Advances, 2014, 4, 25018-25027.	1.7	5
22	Electronegativity estimator built on QTAIMâ€based domains of the bond electron density. Journal of Computational Chemistry, 2014, 35, 978-985.	1.5	9
23	Complementarity of QTAIM and ELF Partitions: Deeper Understanding of the Anomeric Effect. Journal of Chemical Theory and Computation, 2013, 9, 4816-4824.	2.3	12
24	Influence of the O-Protonation in the Oâ•Câ€“O-Me Z Preference. A QTAIM Study. Journal of Physical Chemistry A, 2013, 117, 257-265.	1.1	8
25	Anomeric Effect in Halogenated Methanols: A Quantum Theory of Atoms in Molecules Study. Journal of Physical Chemistry A, 2013, 117, 1641-1650.	1.1	18
26	A QTAIMâ€based energy partitioning for understanding the physical origin of conformational preferences: Application to the Z effect in O=Câ€Xâ€R and related units. Journal of Computational Chemistry, 2012, 33, 2533-2543.	1.5	15
27	An Electronâ€Densityâ€Based Study on the Ionic Reactivity of 1,3â€Azoles. European Journal of Organic Chemistry, 2012, 2012, 2403-2413.	1.2	5
28	Electronic Interpretation of Conformational Preferences in Benzyl Derivatives and Related Compounds. Journal of Physical Chemistry A, 2011, 115, 13088-13095.	1.1	5
29	Influence of the Solvent on the Charge Distribution of Anomeric Compounds. Journal of Physical Chemistry A, 2011, 115, 1964-1970.	1.1	15
30	Hydration Structure of Cocaine and its Metabolites: A Molecular Dynamics Study. Journal of Solution Chemistry, 2011, 40, 656-679.	0.6	1
31	Molecular structure of cyanidin metal complexes: Al(III) versus Mg(II). Theoretical Chemistry Accounts, 2011, 128, 485-495.	0.5	18
32	On the non-planarity of 1,3-dioxole and 1,3-dioxolane. Chemical Physics Letters, 2010, 488, 17-21.	1.2	7
33	Theoretical study of morphine and heroin: Conformational study in gas phase and aqueous solution and electron distribution analysis. International Journal of Quantum Chemistry, 2010, 110, 2472-2482.	1.0	3
34	Evidence for Hydrogen-Bonding-Directed Assembly of Gold Nanorods in Aqueous Solution. Journal of Physical Chemistry Letters, 2010, 1, 1181-1185.	2.1	81
35	A Computational Study on the Acidity Dependence of Radical-Scavenging Mechanisms of Anthocyanidins. Journal of Physical Chemistry B, 2010, 114, 9706-9712.	1.2	62
36	Theoretical study of cocaine and ecgonine methyl ester in gas phase and in aqueous solution. Chemical Physics Letters, 2009, 467, 249-254.	1.2	9

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37	6-Electron exchange function as a simple estimator of aromaticity in large polyaromatic hydrocarbons. Chemical Physics Letters, 2009, 470, 140-146.	1.2	3
38	Electron Density Analysis on the Protonation of Nitriles. Journal of Physical Chemistry A, 2009, 113, 2652-2657.	1.1	16
39	Conformational and Substitution Effects on the Electron Distribution in a Series of Anthocyanidins. Journal of Physical Chemistry A, 2009, 113, 9908-9919.	1.1	19
40	On the Electronic Structure of Cocaine and its Metabolites. Journal of Physical Chemistry A, 2009, 113, 13937-13942.	1.1	9
41	Computational Study on the Stacking Interaction in Catechol Complexes. Journal of Physical Chemistry A, 2009, 113, 11051-11058.	1.1	22
42	The pseudo-Ï€ method examined for the computation of multicenter aromaticity indices. Journal of Mathematical Chemistry, 2008, 43, 111-118.	0.7	27
43	Where is the positive charge of flavylium cations?. Chemical Physics Letters, 2008, 451, 121-126.	1.2	13
44	Interplay between Hydrogen-Bond Formation and Multicenter Ï€-Electron Delocalization: Intramolecular Hydrogen Bonds. Journal of Physical Chemistry A, 2008, 112, 10689-10696.	1.1	28
45	Interplay Between Hydrogen Bond Formation and Multicenter Ï€-Electron Delocalization: Intermolecular Hydrogen Bonds. Journal of Physical Chemistry A, 2008, 112, 7898-7904.	1.1	24
46	Molecular Structure and Antioxidant Properties of Delphinidin. Journal of Physical Chemistry A, 2008, 112, 10614-10623.	1.1	67
47	Conformational study and electron density analysis of 9-[tetrahydropyran-3-yl]purine derivatives. Tetrahedron, 2007, 63, 717-726.	1.0	4
48	A Computational Study on the Stacking Interaction in Quinhydrone. Journal of Physical Chemistry A, 2007, 111, 1998-2001.	1.1	42
49	A Density Functional Theory Study on Pelargonidin. Journal of Physical Chemistry A, 2007, 111, 11100-11109.	1.1	26
50	Revisiting the calculation of condensed Fukui functions using the quantum theory of atoms in molecules. Journal of Chemical Physics, 2007, 126, 234108.	1.2	25
51	Interpretation of Anomeric Effect in the Nâˆ’Câˆ’N Unit with the Quantum Theory of Atoms in Molecules. Journal of Physical Chemistry A, 2007, 111, 8491-8499.	1.1	38
52	Nucleophilicity of Indole Derivatives:Â Activating and Deactivating Effects Based on Proton Affinities and Electron Density Properties. Journal of Physical Chemistry A, 2007, 111, 5557-5562.	1.1	40
53	QTAIMn-center delocalization indices as descriptors of aromaticity in mono and poly heterocycles. Journal of Computational Chemistry, 2007, 28, 127-136.	1.5	104
54	Atoms in molecules interpretation of the anomeric effect in the Oï£¿Cï£¿O unit. Journal of Computational Chemistry, 2007, 28, 1516-1530.	1.5	91

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55	Chemical graph theory andn-center electron delocalization indices: A study on polycyclic aromatic hydrocarbons. Journal of Computational Chemistry, 2007, 28, 1625-1633.	1.5	37
56	Characterization of Pericyclic Reactions Using Multicenter Electron Delocalization Analysis. ChemPhysChem, 2007, 8, 696-702.	1.0	23
57	Approximate transferability in conjugated polyalkenes. Chemical Physics Letters, 2007, 437, 1-7.	1.2	3
58	QTAIM explanation of the anomeric effect in the Oâ€“Câ€“O unit II: 2-Methoxyoxane and 2,2-dimethoxypropane. Chemical Physics Letters, 2007, 443, 22-28.	1.2	18
59	A density functional theory study of the hydrogen bond interactions in glycine dimers. Chemical Physics Letters, 2007, 445, 117-124.	1.2	23
60	QTAIM electron density study of natural chalcones. Chemical Physics Letters, 2007, 446, 1-7.	1.2	14
61	On the Electronic Origin of Strain Energy:â€‰ QTAIM Study of Perfluorocycloalkanes. Journal of Physical Chemistry A, 2006, 110, 11752-11759.	1.1	10
62	Do the Neighboring Residues in a Polypeptide Affect the Electron Distribution of an Amino Acid Significantly? A Quantitative Study Using the Quantum Theory of Atoms in Molecules (QTAIM). Journal of Chemical Information and Modeling, 2006, 46, 2056-2065.	2.5	11
63	On the Electron Donor and the Electrophilic Substitution Activating Abilities of Substituents in Uracil. Journal of Physical Chemistry A, 2006, 110, 5934-5941.	1.1	9
64	Are the hydrogen bonds involving sulfur bases inverse or anomalous?. International Journal of Quantum Chemistry, 2006, 106, 928-934.	1.0	13
65	Do small carboxylic acids present intramolecular hydrogen bond?. Chemical Physics, 2006, 323, 211-217.	0.9	19
66	A charge density analysis on the proximity effect in dicyanoalkanes. Chemical Physics Letters, 2006, 422, 558-564.	1.2	6
67	QTAIM charge density study of natural cinnamic acids. Chemical Physics Letters, 2006, 424, 17-22.	1.2	15
68	QTAIM study of the protonation of indole. Chemical Physics Letters, 2006, 428, 249-254.	1.2	28
69	Explaining the sequence of protonation affinities of cytosine with QTAIM. Chemical Physics Letters, 2006, 428, 255-261.	1.2	20
70	Multicenter delocalization indices vs. properties of the electron density at ring critical points: A study on polycyclic aromatic hydrocarbons. Chemical Physics Letters, 2006, 433, 5-9.	1.2	38
71	A scheme estimating the energy of intramolecular hydrogen bonds in diols. Tetrahedron, 2006, 62, 4243-4252.	1.0	25
72	Local aromaticity study of heterocycles using n-center delocalization indices: the role of aromaticity on the relative stability of position isomers. Tetrahedron, 2006, 62, 12204-12210.	1.0	66

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73	Topological characterisation of intermolecular lithium bonding. Chemical Physics, 2006, 326, 401-408.	0.9	47
74	Hartreeâ€“Fock Energy Partitioning in Terms of Hirshfeld Atoms. ChemPhysChem, 2006, 7, 1294-1305.	1.0	26
75	Charge density analysis of some processes involving intramolecular hydrogen transfer. Tetrahedron, 2005, 61, 819-829.	1.0	6
76	Electron charge redistribution upon hydride addition to carbonylic compounds. Chemical Physics Letters, 2005, 405, 10-17.	1.2	14
77	QTAIM study of the electronic structure and strain energy of fluorine substituted oxiranes and thiiranes. Chemical Physics Letters, 2005, 405, 440-447.	1.2	7
78	QTAIM interpretation of the basicity of substituted anilines. Chemical Physics Letters, 2005, 412, 106-109.	1.2	11
79	Topological study of intramolecular hydrogen bonding in Î²-hydroxyethylperoxy radical and Î²-hydroxyethoxy radical along its dissociation pathway. Physical Chemistry Chemical Physics, 2005, 7, 3290.	1.3	3
80	Quantum Theory of Atoms in Molecules Analysis on the Conformational Preferences of Vinyl Alcohol and Related Ethers. Journal of Physical Chemistry A, 2005, 109, 6985-6989.	1.1	13
81	On the Applicability of Resonance Forms in Pyrimidinic Bases. II. QTAIM Interpretation of the Sequence of Protonation Affinities. Journal of Physical Chemistry A, 2005, 109, 3682-3686.	1.1	20
82	Joint QTAIM and Hirshfeld Study of the Ïƒ and Ï€ Charge Distribution and Electron Delocalization in Carbonyl Compounds:Â A Comparative Study with the Resonance Model. Journal of Physical Chemistry A, 2005, 109, 8624-8631.	1.1	13
83	Theoretical study of the electronic structure of CnSâ€Š(n=1â€“6) thiocumulenes. Journal of Chemical Physics, 2004, 121, 10447-10455.	1.2	17
84	AIM interpretation of the acidity of phenol derivatives. Chemical Physics Letters, 2004, 386, 454-459.	1.2	13
85	AIM charge density study of simple natural phenolic antioxidants. Chemical Physics Letters, 2004, 400, 169-174.	1.2	25
86	Do 1,2-ethanediol and 1,2-dihydroxybenzene present intramolecular hydrogen bond?. Physical Chemistry Chemical Physics, 2004, 6, 4391-4396.	1.3	77
87	Comparison of the AIM and Hirshfeld Totals, Ïƒ, and Ï€ Charge Distributions:Â A Study of Protonation and Hydride Addition Processes. Journal of Physical Chemistry A, 2004, 108, 7050-7055.	1.1	26
88	On the structures of the methanol trimer and their cooperative effects. Chemical Physics Letters, 2003, 381, 22-29.	1.2	45
89	A box-counting-based algorithm for computing Shannon entropy in molecular dynamics simulations. Journal of Computational Chemistry, 2003, 24, 707-713.	1.5	2
90	AIM study on the protonation of methyl oxiranes. Chemical Physics Letters, 2003, 371, 540-547.	1.2	11

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91	Transferability of energies of atoms in organic molecules. Chemical Physics Letters, 2003, 371, 739-743.	1.2	24
92	Theoretical binding enthalpies and topological analysis of complexes of linear and cyclic ethers with Li+, Na+ and K+. Chemical Physics Letters, 2003, 375, 499-505.	1.2	6
93	AIM interpretation of strain energy of oxiranes. Chemical Physics, 2003, 287, 125-135.	0.9	9
94	AIM study on the influence of fluorine atoms on the alkyl chain. Chemical Physics, 2003, 287, 227-236.	0.9	19
95	On the different origin of the stabilisation of oxygen versus sulphur H-bond complexes with water. Chemical Physics, 2003, 291, 73-80.	0.9	22
96	Applicability of Resonance Forms in Pyrimidinic Bases. An AIM Study. Journal of Physical Chemistry A, 2003, 107, 5361-5367.	1.1	33
97	Approximate transferability in alkanols. Computational and Theoretical Chemistry, 2002, 584, 221-234.	1.5	27
98	AIM electron density analysis on the structure and bonding in oxiranes. Computational and Theoretical Chemistry, 2002, 586, 47-56.	1.5	5
99	Topological study on the proximity effect on methylene groups in dimethoxyethers. Computational and Theoretical Chemistry, 2002, 617, 219-224.	1.5	7
100	Electron density characterisation of intermolecular interactions in the formaldehyde dimer and trimer. Chemical Physics, 2002, 281, 11-22.	0.9	33
101	AIM study of pyrimidyl carbocyclic analogues of nucleosides based on cyclopentene rings. International Journal of Quantum Chemistry, 2002, 86, 67-78.	1.0	5
102	Approximate transferability in alkanenitriles. International Journal of Quantum Chemistry, 2002, 86, 190-198.	1.0	23
103	On the effects of electron correlation and conformational changes on the distortion of the charge distribution in alkyl chains. Chemical Physics Letters, 2002, 355, 529-537.	1.2	13
104	Approximate transferability in alkanes revisited. Chemical Physics Letters, 2002, 356, 305-312.	1.2	21
105	Transferability in alkyl monoethers. II. Methyl and methylene fragments. Journal of Chemical Physics, 2001, 115, 1264-1273.	1.2	42
106	Electron density analysis of small ring ethers. Tetrahedron, 2001, 57, 9415-9422.	1.0	23
107	An electron density analysis of the proximity effect in linear alkyl diethers. Chemical Physics Letters, 2001, 345, 445-452.	1.2	10
108	On the perfluorination of alkyl ethers. An electron density study under the AIM approach. Computational and Theoretical Chemistry, 2001, 546, 63-72.	1.5	27

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109	An AIM study on the effects of position isomery in long-chain alkanols. Computational and Theoretical Chemistry, 2001, 572, 223-233.	1.5	8
110	The evolution of the atomic and bond properties during internal rotation of the hydrazine molecule. Journal of Molecular Structure, 2000, 556, 69-76.	1.8	7
111	Evolution of the Atomic and Bond Properties of Hydrogen Peroxide During Internal Rotation. Structural Chemistry, 2000, 11, 9-13.	1.0	10
112	Transferability in aldehydes and ketones. II. Alkyl chains. Journal of Chemical Physics, 2000, 113, 1492-1500.	1.2	37
113	AIM study on the transferability of the oxygen atom in linear ethers. Canadian Journal of Chemistry, 2000, 78, 1535-1543.	0.6	35
114	Topological Analysis of Fluorinated Dimethyl Ethers and Their Protonated Forms. Journal of Physical Chemistry A, 2000, 104, 12006-12013.	1.1	23
115	Effect of protonation on the atomic and bond properties of the carbonyl group in aldehydes and ketones. Chemical Physics, 1999, 243, 17-26.	0.9	23
116	Atomic and bond properties in functionalized esters and amides. Journal of Computational Chemistry, 1999, 20, 1444-1454.	1.5	8
117	The transferability of the carbonyl group in aldehydes and ketones. Journal of Chemical Physics, 1999, 110, 6606-6616.	1.2	60
118	Quantum mechanical characterisation of functional groups for molecular solution theories using Bader fragments. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 3437-3443.	1.7	18
119	Conformational analysis of model compounds of vitamin D by theoretical calculations. Journal of Computational Chemistry, 1997, 18, 1647-1655.	1.5	6
120	Structure-activity relationships in verapamil and analogues using molecular mechanics calculations. International Journal of Pharmaceutics, 1992, 79, 199-203.	2.6	4
121	Ab initio conformational studies of peroxides. Computational and Theoretical Chemistry, 1991, 235, 25-37.	1.5	6
122	An ab initio conformational analysis of isobutylamine and diisopropylamine. Computational and Theoretical Chemistry, 1991, 251, 319-326.	1.5	1
123	An ab initio gradient study of ethylhydrazine. Computational and Theoretical Chemistry, 1990, 206, 49-66.	1.5	5
124	Ab initio gradient conformational analysis of polyazocyclohexanes:1,4-diazocyclohexane, 1,3-diazocyclohexane and 1,3,5-triazocyclohexane. Computational and Theoretical Chemistry, 1990, 205, 223-234.	1.5	8
125	Ab initio studies of molecules with N-C-O units. Computational and Theoretical Chemistry, 1990, 205, 235-244.	1.5	9
126	Ab initio-gradient optimized molecular geometry and conformational analysis of 2-methoxyethanol at the 4-21G level. Computational and Theoretical Chemistry, 1989, 188, 95-104.	1.5	17

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127	An ab initio gradient study of trimethylhydrazine. Computational and Theoretical Chemistry, 1989, 184, 311-322.	1.5	1
128	AB initio gradient optimized molecular geometry and conformational analysis of 1,2-propanediol at the 4-21G level. Computational and Theoretical Chemistry, 1989, 184, 323-342.	1.5	22
129	Study of the geometric trends and rotational constants of 1-fluoro-2-propanol and 2-fluoropropanol by Ab Initio calculations. Tetrahedron Computer Methodology, 1989, 2, 85-92.	0.2	1
130	Conformational analysis of polyfunctional amino compounds by molecular mechanics.. Journal of Molecular Structure, 1989, 193, 263-277.	1.8	18
131	Conformational analysis of polyfunctional amino compounds by molecular mechanics. Journal of Molecular Structure, 1989, 195, 89-101.	1.8	9
132	A study of the molecular structure of cocaine using molecular mechanics and NMR. Journal of Molecular Structure, 1989, 195, 325-333.	1.8	10
133	Conformational analysis of vitamin D3 derivatives by molecular mechanics. Journal of Molecular Structure, 1989, 213, 297-307.	1.8	3
134	Molecular mechanics of peroxides. I. Parametrization and conformational analysis of linear compounds. Journal of Computational Chemistry, 1988, 9, 851-860.	1.5	18
135	Conformational analysis of polyfunctional aminic compounds by molecular mechanics. Journal of Molecular Structure, 1988, 176, 89-105.	1.8	14
136	Ab initio-gradient optimized molecular geometry and conformational analysis of 1,3-propanediol at the 4-21G level. Computational and Theoretical Chemistry, 1988, 181, 149-167.	1.5	25
137	Conformational analysis of 5Z- and 5E-vitamin D3 dihydroderivatives by molecular mechanics. Computational and Theoretical Chemistry, 1988, 168, 125-133.	1.5	6
138	Complete structural analysis of cyclic polyhalogenated monoterpenes. A force field 2-dimensional NMR study. Journal of Organic Chemistry, 1986, 51, 4970-4973.	1.7	4
139	Conformational analysis of divinylketones by molecular mechanics (MMPI). Computational and Theoretical Chemistry, 1986, 136, 351-359.	1.5	1