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	QTAIMn-center delocalization indices as descriptors of aromaticity in mono and poly heterocycles. Journal of Computational Chemistry, 2007, 28, 127-136.	1.5	104
2	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
3	Evidence for Hydrogen-Bonding-Directed Assembly of Gold Nanorods in Aqueous Solution. Journal of Physical Chemistry Letters, 2010, 1, 1181-1185.	2.1	81
4	Do 1,2-ethanediol and 1,2-dihydroxybenzene present intramolecular hydrogen bond?. Physical Chemistry Chemical Physics, 2004, 6, 4391-4396.	1.3	77
5	Molecular Structure and Antioxidant Properties of Delphinidin. Journal of Physical Chemistry A, 2008, 112, 10614-10623.	1.1	67
6	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
7	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
8	The transferability of the carbonyl group in aldehydes and ketones. Journal of Chemical Physics, 1999, 110, 6606-6616.	1.2	60
9	Topological characterisation of intermolecular lithium bonding. Chemical Physics, 2006, 326, 401-408.	0.9	47
10	On the structures of the methanol trimer and their cooperative effects. Chemical Physics Letters, 2003, 381, 22-29.	1.2	45
11	Transferability in alkyl monoethers. II. Methyl and methylene fragments. Journal of Chemical Physics, 2001, 115, 1264-1273.	1.2	42
12	A Computational Study on the Stacking Interaction in Quinhydrone. Journal of Physical Chemistry A, 2007, 111, 1998-2001.	1.1	42
13	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
14	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
15	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
16	Transferability in aldehydes and ketones. II. Alkyl chains. Journal of Chemical Physics, 2000, 113, 1492-1500.	1.2	37
17	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
18	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

#	Article	IF	Citations
19	AIM study on the transferability of the oxygen atom in linear ethers. Canadian Journal of Chemistry, 2000, 78, 1535-1543.	0.6	35
20	Electron density characterisation of intermolecular interactions in the formaldehyde dimer and trimer. Chemical Physics, 2002, 281, 11-22.	0.9	33
21	Applicability of Resonance Forms in Pyrimidinic Bases. An AIM Study. Journal of Physical Chemistry A, 2003, 107, 5361-5367.	1.1	33
22	QTAIM study of the protonation of indole. Chemical Physics Letters, 2006, 428, 249-254.	1.2	28
23	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
24	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
25	Approximate transferability in alkanols. Computational and Theoretical Chemistry, 2002, 584, 221-234.	1.5	27
26	The pseudo-Ï€ method examined for the computation of multicenter aromaticity indices. Journal of Mathematical Chemistry, 2008, 43, 111-118.	0.7	27
27	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
28	Hartreeâ€“Fock Energy Partitioning in Terms of Hirshfeld Atoms. ChemPhysChem, 2006, 7, 1294-1305.	1.0	26
29	A Density Functional Theory Study on Pelargonidin. Journal of Physical Chemistry A, 2007, 111, 11100-11109.	1.1	26
30	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
31	AIM charge density study of simple natural phenolic antioxidants. Chemical Physics Letters, 2004, 400, 169-174.	1.2	25
32	A scheme estimating the energy of intramolecular hydrogen bonds in diols. Tetrahedron, 2006, 62, 4243-4252.	1.0	25
33	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
34	Transferability of energies of atoms in organic molecules. Chemical Physics Letters, 2003, 371, 739-743.	1.2	24
35	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
36	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

#	Article	IF	Citations
37	Topological Analysis of Fluorinated Dimethyl Ethers and Their Protonated Forms. Journal of Physical Chemistry A, 2000, 104, 12006-12013.	1.1	23
38	Electron density analysis of small ring ethers. Tetrahedron, 2001, 57, 9415-9422.	1.0	23
39	Approximate transferability in alkanenitriles. International Journal of Quantum Chemistry, 2002, 86, 190-198.	1.0	23
40	Characterization of Pericyclic Reactions Using Multicenter Electron Delocalization Analysis. ChemPhysChem, 2007, 8, 696-702.	1.0	23
41	A density functional theory study of the hydrogen bond interactions in glycine dimers. Chemical Physics Letters, 2007, 445, 117-124.	1.2	23
42	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
43	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
44	Computational Study on the Stacking Interaction in Catechol Complexes. Journal of Physical Chemistry A, 2009, 113, 11051-11058.	1.1	22
45	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
46	Approximate transferability in alkanes revisited. Chemical Physics Letters, 2002, 356, 305-312.	1.2	21
47	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
48	Explaining the sequence of protonation affinities of cytosine with QTAIM. Chemical Physics Letters, 2006, 428, 255-261.	1.2	20
49	AIM study on the influence of fluorine atoms on the alkyl chain. Chemical Physics, 2003, 287, 227-236.	0.9	19
50	Do small carboxylic acids present intramolecular hydrogen bond?. Chemical Physics, 2006, 323, 211-217.	0.9	19
51	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
52	Molecular mechanics of peroxides. I. Parametrization and conformational analysis of linear compounds. Journal of Computational Chemistry, 1988, 9, 851-860.	1.5	18
53	Conformational analysis of polyfunctional amino compounds by molecular mechanics.. Journal of Molecular Structure, 1989, 193, 263-277.	1.8	18
54	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

#	Article	IF	Citations
55	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
56	Molecular structure of cyanidin metal complexes: Al(III) versus Mg(II). Theoretical Chemistry Accounts, 2011, 128, 485-495.	0.5	18
57	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
58	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
59	Theoretical study of the electronic structure of CnSâ€Š(n=1â€“6) thiocumulenes. Journal of Chemical Physics, 2004, 121, 10447-10455.	1.2	17
60	Electron Density Analysis on the Protonation of Nitriles. Journal of Physical Chemistry A, 2009, 113, 2652-2657.	1.1	16
61	QTAIM charge density study of natural cinnamic acids. Chemical Physics Letters, 2006, 424, 17-22.	1.2	15
62	Influence of the Solvent on the Charge Distribution of Anomeric Compounds. Journal of Physical Chemistry A, 2011, 115, 1964-1970.	1.1	15
63	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
64	Conformational analysis of polyfunctional aminic compounds by molecular mechanics. Journal of Molecular Structure, 1988, 176, 89-105.	1.8	14
65	Electron charge redistribution upon hydride addition to carbonylic compounds. Chemical Physics Letters, 2005, 405, 10-17.	1.2	14
66	QTAIM electron density study of natural chalcones. Chemical Physics Letters, 2007, 446, 1-7.	1.2	14
67	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
68	AIM interpretation of the acidity of phenol derivatives. Chemical Physics Letters, 2004, 386, 454-459.	1.2	13
69	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
70	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
71	Are the hydrogen bonds involving sulfur bases inverse or anomalous?. International Journal of Quantum Chemistry, 2006, 106, 928-934.	1.0	13
72	Where is the positive charge of flavylium cations?. Chemical Physics Letters, 2008, 451, 121-126.	1.2	13

#	Article	IF	Citations
73	Principal component analysis of Mn(salen) catalysts. Physical Chemistry Chemical Physics, 2014, 16, 25364-25376.	1.3	13
74	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
75	Charge distribution in Mn(salen) complexes. International Journal of Quantum Chemistry, 2014, 114, 525-533.	1.0	12
76	AIM study on the protonation of methyl oxiranes. Chemical Physics Letters, 2003, 371, 540-547.	1.2	11
77	QTAIM interpretation of the basicity of substituted anilines. Chemical Physics Letters, 2005, 412, 106-109.	1.2	11
78	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
79	Complexation of common metal cations by cyanins: Binding affinity and molecular structure. International Journal of Quantum Chemistry, 2019, 119, e25834.	1.0	11
80	A study of the molecular structure of cocaine using molecular mechanics and NMR. Journal of Molecular Structure, 1989, 195, 325-333.	1.8	10
81	Evolution of the Atomic and Bond Properties of Hydrogen Peroxide During Internal Rotation. Structural Chemistry, 2000, 11, 9-13.	1.0	10
82	An electron density analysis of the proximity effect in linear alkyl diethers. Chemical Physics Letters, 2001, 345, 445-452.	1.2	10
83	On the Electronic Origin of Strain Energy:â€‰ QTAIM Study of Perfluorocycloalkanes. Journal of Physical Chemistry A, 2006, 110, 11752-11759.	1.1	10
84	Effects of Axial Coordination on Immobilized Mn(salen) Catalysts. Journal of Physical Chemistry A, 2014, 118, 10788-10796.	1.1	10
85	Conformational analysis of polyfunctional amino compounds by molecular mechanics. Journal of Molecular Structure, 1989, 195, 89-101.	1.8	9
86	Ab initio studies of molecules with N-C-O units. Computational and Theoretical Chemistry, 1990, 205, 235-244.	1.5	9
87	AIM interpretation of strain energy of oxiranes. Chemical Physics, 2003, 287, 125-135.	0.9	9
88	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
89	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
90	On the Electronic Structure of Cocaine and its Metabolites. Journal of Physical Chemistry A, 2009, 113, 13937-13942.	1.1	9

#	Article	IF	Citations
91	Electronegativity estimator built on QTAIMâ€based domains of the bond electron density. Journal of Computational Chemistry, 2014, 35, 978-985.	1.5	9
92	How Electronic Excitation Can be Used to Inhibit Some Mechanisms Associated to Substituent Effects. ChemPhysChem, 2016, 17, 2666-2671.	1.0	9
93	Roots of Acetate-Vanadium Linkage Isomerism: A QTAIM Study. Inorganic Chemistry, 2016, 55, 3653-3662.	1.9	9
94	Driving Forces in the Sharpless Epoxidation Reaction: A Coupled AIMD/QTAIM Study. Inorganic Chemistry, 2017, 56, 2124-2134.	1.9	9
95	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
96	Atomic and bond properties in functionalized esters and amides. Journal of Computational Chemistry, 1999, 20, 1444-1454.	1.5	8
97	An AIM study on the effects of position isomery in long-chain alkanols. Computational and Theoretical Chemistry, 2001, 572, 223-233.	1.5	8
98	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
99	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
100	Topological study on the proximity effect on methylene groups in dimethoxyethers. Computational and Theoretical Chemistry, 2002, 617, 219-224.	1.5	7
101	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
102	On the non-planarity of 1,3-dioxole and 1,3-dioxolane. Chemical Physics Letters, 2010, 488, 17-21.	1.2	7
103	Conformational analysis of 5Z- and 5E-vitamin D3 dihydroderivatives by molecular mechanics. Computational and Theoretical Chemistry, 1988, 168, 125-133.	1.5	6
104	Ab initio conformational studies of peroxides. Computational and Theoretical Chemistry, 1991, 235, 25-37.	1.5	6
105	Conformational analysis of model compounds of vitamin D by theoretical calculations. Journal of Computational Chemistry, 1997, 18, 1647-1655.	1.5	6
106	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
107	Charge density analysis of some processes involving intramolecular hydrogen transfer. Tetrahedron, 2005, 61, 819-829.	1.0	6
108	A charge density analysis on the proximity effect in dicyanoalkanes. Chemical Physics Letters, 2006, 422, 558-564.	1.2	6

#	Article	IF	Citations
109	An ab initio gradient study of ethylhydrazine. Computational and Theoretical Chemistry, 1990, 206, 49-66.	1.5	5
110	AIM electron density analysis on the structure and bonding in oxiranes. Computational and Theoretical Chemistry, 2002, 586, 47-56.	1.5	5
111	AIM study of pyrimidyl carbocyclic analogues of nucleosides based on cyclopentene rings. International Journal of Quantum Chemistry, 2002, 86, 67-78.	1.0	5
112	Electronic Interpretation of Conformational Preferences in Benzyl Derivatives and Related Compounds. Journal of Physical Chemistry A, 2011, 115, 13088-13095.	1.1	5
113	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
114	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
115	Revisiting Lewis dot structure weightings: a pair density perspective. Physical Chemistry Chemical Physics, 2015, 17, 7424-7434.	1.3	5
116	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
117	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
118	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
119	Structure-activity relationships in verapamil and analogues using molecular mechanics calculations. International Journal of Pharmaceutics, 1992, 79, 199-203.	2.6	4
120	Conformational study and electron density analysis of 9-[tetrahydropyran-3-yl]purine derivatives. Tetrahedron, 2007, 63, 717-726.	1.0	4
121	When valence bond wave functions are analyzed through QTAIM: Conceptual incompatibilities in H2. Chemical Physics Letters, 2015, 618, 83-88.	1.2	4
122	Computational Studies on Conformation, Electron Density Distributions, and Antioxidant Properties of Anthocyanidins. Methods in Molecular Biology, 2015, 1208, 257-276.	0.4	4
123	Conformational analysis of vitamin D3 derivatives by molecular mechanics. Journal of Molecular Structure, 1989, 213, 297-307.	1.8	3
124	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
125	Approximate transferability in conjugated polyalkenes. Chemical Physics Letters, 2007, 437, 1-7.	1.2	3
126	6-Electron exchange function as a simple estimator of aromaticity in large polyaromatic hydrocarbons. Chemical Physics Letters, 2009, 470, 140-146.	1.2	3

#	Article	IF	Citations
127	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
128	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
129	Chiroptical Symmetry Analysis of Trianglimines: A Case Study. Symmetry, 2019, 11, 1245.	1.1	3
130	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
131	A box-counting-based algorithm for computing Shannon entropy in molecular dynamics simulations. Journal of Computational Chemistry, 2003, 24, 707-713.	1.5	2
132	On the structure of Zn(II) and Cu(II) cyanin complexes in aqueous solution. Structural Chemistry, 2014, 25, 1647-1657.	1.0	2
133	Exploring the versatility of the gCH topological electronegativity estimator. Computational and Theoretical Chemistry, 2015, 1053, 85-89.	1.1	2
134	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
135	Conformational analysis of divinylketones by molecular mechanics (MMPI). Computational and Theoretical Chemistry, 1986, 136, 351-359.	1.5	1
136	An ab initio gradient study of trimethylhydrazine. Computational and Theoretical Chemistry, 1989, 184, 311-322.	1.5	1
137	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
138	An ab initio conformational analysis of isobutylamine and diisopropylamine. Computational and Theoretical Chemistry, 1991, 251, 319-326.	1.5	1
139	Hydration Structure of Cocaine and its Metabolites: A Molecular Dynamics Study. Journal of Solution Chemistry, 2011, 40, 656-679.	0.6	1