Ana M Grana

List of Publications by Year
in descending order

44 papers	1,054 citations	471371 17 h-index	414303 32 g-index
46 all docs	46 docs citations	46 times ranked	1247 citing authors

#	Article	IF	Citations
1	Analysis of Electronic Transitions as the Difference of Electron Attachment and Detachment Densities. The Journal of Physical Chemistry, 1995, 99, 14261-14270.	2.9	288
2	Do 1,2-ethanediol and 1,2-dihydroxybenzene present intramolecular hydrogen bond?. Physical Chemistry Chemical Physics, 2004, 6, 4391-4396.	1.3	77
3	The transferability of the carbonyl group in aldehydes and ketones. Journal of Chemical Physics, 1999, 110, 6606-6616.	1.2	60
4	On the structures of the methanol trimer and their cooperative effects. Chemical Physics Letters, 2003, 381, 22-29.	1.2	45
5	Ab Initio Calculations of Singlet and Triplet Excited States of Chlorine Nitrate and Nitric Acid. The Journal of Physical Chemistry, 1995, 99, 3493-3502.	2.9	44
6	Aromaticity in spin-polarized systems: Can rings be simultaneously alpha aromatic and beta antiaromatic?. Journal of Chemical Physics, 2008, 129, 164114.	1.2	39
7	Transferability in aldehydes and ketones. II. Alkyl chains. Journal of Chemical Physics, 2000, 113, 1492-1500.	1.2	37
8	Electron density characterisation of intermolecular interactions in the formaldehyde dimer and trimer. Chemical Physics, 2002, 281, 11-22.	0.9	33
9	How Does Aromaticity Rule the Thermodynamic Stability of Hydroporphyrins?. Chemistry - A European Journal, 2011, 17, 3274-3286.	1.7	31
10	Approximate transferability in alkanols. Computational and Theoretical Chemistry, 2002, 584, 221-234.	1.5	27
11	AIM charge density study of simple natural phenolic antioxidants. Chemical Physics Letters, 2004, 400, 169-174.	1.2	25
12	Transferability of energies of atoms in organic molecules. Chemical Physics Letters, 2003, 371, 739-743.	1.2	24
13	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
14	Approximate transferability in alkanenitriles. International Journal of Quantum Chemistry, 2002, 86, 190-198.	1.0	23
15	Blue-shifting hydrogen bond in the benzeneâ€“benzene and benzeneâ€“naphthalene complexes. Journal of Computational Chemistry, 2007, 28, 540-546.	1.5	20
16	AIM study on the influence of fluorine atoms on the alkyl chain. Chemical Physics, 2003, 287, 227-236.	0.9	19
17	Theoretical study of the electronic structure of CnSâ€Š(n=1â€“6) thiocumulenes. Journal of Chemical Physics, 2004, 121, 10447-10455.	1.2	17
18	Ab initio study of the structure and tautomerism of internally hydrogen-bonded aromatic carbonyls: Salicylaldehyde and o-hydroxyacetophenone. Structural Chemistry, 1991, 2, 575-580.	1.0	16

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19	Electron Density Analysis on the Protonation of Nitriles. Journal of Physical Chemistry A, 2009, 113, 2652-2657.	1.1	16
20	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
21	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
22	AIM interpretation of the acidity of phenol derivatives. Chemical Physics Letters, 2004, 386, 454-459.	1.2	13
23	Structure and tautomerism of 7-azaindole in the ground and excited states. Computational and Theoretical Chemistry, 1999, 466, 145-153.	1.5	11
24	QTAIM interpretation of the basicity of substituted anilines. Chemical Physics Letters, 2005, 412, 106-109.	1.2	11
25	Study of electron transport in polybenzenoid chains covalently attached to gold atoms through unsaturated methylene linkers. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	11
26	Synthesis of Novel Dinuclear N-Substituted 4-(Dimethylamino)benzaldehyde Thiosemicarbazonates of Rhenium(I): Formation of Four- and/or Five-Membered Chelate Rings, Conformational Analysis, and Reactivity. Inorganic Chemistry, 2020, 59, 14101-14117.	1.9	11
27	Evolution of the Atomic and Bond Properties of Hydrogen Peroxide During Internal Rotation. Structural Chemistry, 2000, 11, 9-13.	1.0	10
28	A semiempirical AM1 conformational study of 3'-substituted deoxythymidines. Computational and Theoretical Chemistry, 1993, 288, 207-214.	1.5	9
29	Atomic and bond properties in functionalized esters and amides. Journal of Computational Chemistry, 1999, 20, 1444-1454.	1.5	8
30	An AIM study on the effects of position isomery in long-chain alkanols. Computational and Theoretical Chemistry, 2001, 572, 223-233.	1.5	8
31	Structural study of mono-, di- and tetranuclear complexes of the {Re(CO)₃}⁺ fragment with thiosemicarbazone/thiosemicarbazonate ligands containing benzothiazole or benzoxazole groups. CrystEngComm, 2018, 20, 4781-4792.	1.3	8
32	Correlation between the anti-HIV activity and electrostatic properties of 3â€²-substituted deoxythymidines. Computational and Theoretical Chemistry, 1995, 334, 37-43.	1.5	7
33	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
34	Structural Study of Methane Hydrate. Structural Chemistry, 2007, 18, 649-652.	1.0	7
35	Semiempirical (AM1) and ab initio calculations of 2-X-adenine (X = H, F, Cl) and Î²-D-1-amino-2,3-didehydro-1,2,3-trideoxyribofuranose. Computational and Theoretical Chemistry, 1993, 280, 211-222.	1.5	6
36	Charge density analysis of some processes involving intramolecular hydrogen transfer. Tetrahedron, 2005, 61, 819-829.	1.0	6

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37	Supramolecular Synthesis and Experimental and Theoretical Studies of Cocrystal Systems Based on Resorcinol-Thiosemicarbazones and N,Nâ€²-Divergent Dipyridines. Crystal Growth and Design, 2017, 17, 3338-3349.	1.4	6
38	Stacking and hydrogen bond interactions between adenine and gallic acid. Journal of Molecular Modeling, 2013, 19, 5293-5299.	0.8	4
39	Ab initio study of the structure and tautomerism in 7-hydroxy-1-indanone. Computational and Theoretical Chemistry, 1991, 226, 303-306.	1.5	3
40	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
41	Rhenium(I) carbonyl complexes bearing the alkenylphosphinite ligand Ph2POCH2CH CH2. Polyhedron, 2020, 176, 114288.	1.0	2
42	Theoretical study of the complexes of light-gated corannulene tweezers with fullerene. Structural Chemistry, 2020, 31, 1331-1337.	1.0	1
43	Allenylidene and diazoalkane complexes of a half-sandwich mixed phosphine â€“ phosphinite ruthenium fragment. Inorganica Chimica Acta, 2021, 519, 120277.	1.2	1
44	USING â€œFLIPPED CLASSROOMâ€œ STRATEGIES TO TEACH UNDERGRADUATE COURSES OF QUANTUM CHEMISTRY. APPLICATION TO A MODIFIED HÃœCKEL METHOD INCLUDING A PARTIAL OVERLAP. EDULEARN Proceedings, 2020, , .	0.0	0