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	Allenylidene and diazoalkane complexes of a half-sandwich mixed phosphine â€“ phosphinite ruthenium fragment. Inorganica Chimica Acta, 2021, 519, 120277.	1.2	1
2	Rhenium(I) carbonyl complexes bearing the alkenylphosphinite ligand Ph2POCH2CH CH2. Polyhedron, 2020, 176, 114288.	1.0	2
3	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
4	Theoretical study of the complexes of light-gated corannulene tweezers with fullerene. Structural Chemistry, 2020, 31, 1331-1337.	1.0	1
5	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
6	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
7	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
8	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
9	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
10	Stacking and hydrogen bond interactions between adenine and gallic acid. Journal of Molecular Modeling, 2013, 19, 5293-5299.	0.8	4
11	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
12	How Does Aromaticity Rule the Thermodynamic Stability of Hydroporphyrins?. Chemistry - A European Journal, 2011, 17, 3274-3286.	1.7	31
13	Electron Density Analysis on the Protonation of Nitriles. Journal of Physical Chemistry A, 2009, 113, 2652-2657.	1.1	16
14	Aromaticity in spin-polarized systems: Can rings be simultaneously alpha aromatic and beta antiaromatic?. Journal of Chemical Physics, 2008, 129, 164114.	1.2	39
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	Structural Study of Methane Hydrate. Structural Chemistry, 2007, 18, 649-652.	1.0	7
17	Charge density analysis of some processes involving intramolecular hydrogen transfer. Tetrahedron, 2005, 61, 819-829.	1.0	6
18	QTAIM interpretation of the basicity of substituted anilines. Chemical Physics Letters, 2005, 412, 106-109.	1.2	11

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19	Theoretical study of the electronic structure of CnSâ€Š(n=1â€“6) thiocumulenes. Journal of Chemical Physics, 2004, 121, 10447-10455.	1.2	17
20	AIM interpretation of the acidity of phenol derivatives. Chemical Physics Letters, 2004, 386, 454-459.	1.2	13
21	AIM charge density study of simple natural phenolic antioxidants. Chemical Physics Letters, 2004, 400, 169-174.	1.2	25
22	Do 1,2-ethanediol and 1,2-dihydroxybenzene present intramolecular hydrogen bond?. Physical Chemistry Chemical Physics, 2004, 6, 4391-4396.	1.3	77
23	On the structures of the methanol trimer and their cooperative effects. Chemical Physics Letters, 2003, 381, 22-29.	1.2	45
24	Transferability of energies of atoms in organic molecules. Chemical Physics Letters, 2003, 371, 739-743.	1.2	24
25	AIM study on the influence of fluorine atoms on the alkyl chain. Chemical Physics, 2003, 287, 227-236.	0.9	19
26	Approximate transferability in alkanols. Computational and Theoretical Chemistry, 2002, 584, 221-234.	1.5	27
27	Electron density characterisation of intermolecular interactions in the formaldehyde dimer and trimer. Chemical Physics, 2002, 281, 11-22.	0.9	33
28	Approximate transferability in alkanenitriles. International Journal of Quantum Chemistry, 2002, 86, 190-198.	1.0	23
29	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
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	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
32	Evolution of the Atomic and Bond Properties of Hydrogen Peroxide During Internal Rotation. Structural Chemistry, 2000, 11, 9-13.	1.0	10
33	Transferability in aldehydes and ketones. II. Alkyl chains. Journal of Chemical Physics, 2000, 113, 1492-1500.	1.2	37
34	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
35	Structure and tautomerism of 7-azaindole in the ground and excited states. Computational and Theoretical Chemistry, 1999, 466, 145-153.	1.5	11
36	Atomic and bond properties in functionalized esters and amides. Journal of Computational Chemistry, 1999, 20, 1444-1454.	1.5	8

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37	The transferability of the carbonyl group in aldehydes and ketones. Journal of Chemical Physics, 1999, 110, 6606-6616.	1.2	60
38	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
39	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
40	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
41	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
42	A semiempirical AM1 conformational study of 3'-substituted deoxythymidines. Computational and Theoretical Chemistry, 1993, 288, 207-214.	1.5	9
43	Ab initio study of the structure and tautomerism in 7-hydroxy-1-indanone. Computational and Theoretical Chemistry, 1991, 226, 303-306.	1.5	3
44	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