Diego F S Paschoal

List of Publications by Year
in descending order

30 papers	395 citations	758635 12 h-index	794141 19 g-index
30 all docs	30 docs citations	30 times ranked	592 citing authors

#	Article	IF	Citations
1	Adsorption study of antibiotics on silver nanoparticle surfaces by surface-enhanced Raman scattering spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 979-985.	2.0	43
2	The role of the basis set and the level of quantum mechanical theory in the prediction of the structure and reactivity of cisplatin. Journal of Computational Chemistry, 2012, 33, 2292-2302.	1.5	39
3	Simultaneous determination of aspartame, cyclamate, saccharin and acesulfame-K in powder tabletop sweeteners by FT-Raman spectroscopy associated with the multivariate calibration: PLS, iPLS and siPLS models were compared. Food Research International, 2017, 99, 106-114.	2.9	28
4	Gold(I) complexes with aryl-thiosemicarbazones: Molecular modeling, synthesis, cytotoxicity and TrxR inhibition. Polyhedron, 2017, 132, 95-104.	1.0	27
5	Ligand Exchange Reaction of Au(I) R-N-Heterocyclic Carbene Complexes with Cysteine. Journal of Physical Chemistry A, 2016, 120, 2250-2259.	1.1	26
6	Predicting Ptâ€195 NMR chemical shift using new relativistic allâ€electron basis set. Journal of Computational Chemistry, 2016, 37, 2360-2373.	1.5	24
7	Platinum(II) and palladium(II) aryl-thiosemicarbazone complexes: synthesis, characterization, molecular modeling, cytotoxicity, and antimicrobial activity. Journal of Coordination Chemistry, 2014, 67, 956-968.	0.8	20
8	Assessing the quantum mechanical level of theory for prediction of linear and nonlinear optical properties of push-pull organic molecules. Journal of Molecular Modeling, 2013, 19, 2079-2090.	0.8	18
9	Ab initio calculation of electric properties for the BH, CO, CS and N2 molecules. Computational and Theoretical Chemistry, 2009, 913, 200-206.	1.5	15
10	Exploring the potential energy surface for interaction of a trichloro(diethylenetriamine)gold(III) complex with strong nucleophiles. Chemical Physics Letters, 2012, 548, 64-70.	1.2	14
11	Exploring the Potential Energy Surface for the Interaction of Sterically Hindered Trichloro(diethylenetriamine)gold(III) Complexes with Water. Journal of Physical Chemistry A, 2012, 116, 11015-11024.	1.1	14
12	Computational protocol to predict hyperpolarizabilities of large Ï€-conjugated organic pushâ€“pull molecules. Organic Electronics, 2016, 28, 111-117.	1.4	13
13	Non-centrosymmetric crystals of newN-benzylideneaniline derivatives as potential materials for non-linear optics. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2015, 71, 416-426.	0.5	12
14	The adsorption of rifampicin on gold or silver surfaces mediated by 2-mercaptoethanol investigated by surface-enhanced Raman scattering spectroscopy. Vibrational Spectroscopy, 2016, 86, 75-80.	1.2	12
15	Reactivity of the [Au(C^N^C)Cl] complex in the presence of H2O and N-, S- and Se-containing nucleophiles: a DFT study. Journal of Biological Inorganic Chemistry, 2018, 23, 1283-1293.	1.1	10
16	NLOâ€X (Xâ€‰=â€‰Iâ€“III): New Gaussian basis sets for prediction of linear and nonlinear electric properties. International Journal of Quantum Chemistry, 2014, 114, 796-804.	1.0	9
17	Structure and redox stability of [Au(III)(X^N^X)PR3] complexes (Xâ€¯=â€¯C or N) in aqueous solution: The role of phosphine auxiliary ligand. Journal of Inorganic Biochemistry, 2019, 200, 110804.	1.5	9
18	Nonrelativistic protocol for calculating the 1J(195Pt-15N) coupling constant in Pt(II)-complexes using all-electron Gaussian basis-set. Chemical Physics Letters, 2020, 745, 137279.	1.2	9

#	Article	IF	Citations
19	Predicting standard reduction potential for anticancer Au(III)-complexes: A DFT study. Computational and Theoretical Chemistry, 2017, 1108, 86-92.	1.1	8
20	Basis Sets for Heavy Atoms. Lecture Notes in Quantum Chemistry II, 2021, , 183-214.	0.3	7
21	A SERS investigation of antimicrobial adsorption on silver nanoparticles as mediated by surface modifiers. Journal of Raman Spectroscopy, 2017, 48, 789-794.	1.2	6
22	Role of the Enzymatic Environment in the Reactivity of the Au^{III}-C^N^C Anticancer Complexes. Inorganic Chemistry, 2021, 60, 3181-3195.	1.9	6
23	Vibrational frequencies and intramolecular force constants for cisplatin: assessing the role of the platinum basis set and relativistic effects. Journal of Molecular Modeling, 2021, 27, 322.	0.8	6
24	Antivirals virtual screening to SARS-CoV-2 non-structural proteins. Journal of Biomolecular Structure and Dynamics, 2022, 40, 8989-9003.	2.0	5
25	Gaussian basis sets for ab initio calculation of NLO properties of polyatomic molecules. Journal of Computational Methods in Sciences and Engineering, 2010, 10, 239-256.	0.1	4
26	¹H and ¹⁹⁵Pt NMR prediction for inclusion compounds formed by cisplatin and oxidized carbon nanostructures. RSC Advances, 2021, 11, 599-611.	1.7	4
27	Predicting Pt-195 NMR Chemical Shift and 1J(195Pt-31P) Coupling Constant for Pt(0) Complexes Using the NMR-DKH Basis Sets. Magnetochemistry, 2021, 7, 148.	1.0	4
28	Predicting the structure and NMR coupling constant ¹J(¹²⁹Xeâ€“¹⁹F) of XeF₆ using quantum mechanics methods. Physical Chemistry Chemical Physics, 2021, 23, 7240-7246.	1.3	2
29	Microwave-assisted synthesis of a new fluorinated Biphenyl-Schiff base with potential application in nonlinear optical / SÃntese assistida por micro-ondas de uma nova Bifenil-Base de Schiff Fluorada com potencial aplicaÃ§Ã£o em Ã³ptica nÃ£o linear. Brazilian Journal of Development, 2021, 7, .	0.0	1
30	Structural Analysis of High-Spin States of S0-S4 at OEC Complex: A Theoretical Approach of Small Models. Journal of the Brazilian Chemical Society, 2016, , .	0.6	0