Nivan Bezerra da Costa Junior

List of Publications by Year
in descending order

58 papers	1,682 citations	304602 22 h-index	302012 39 g-index
58 all docs	58 docs citations	58 times ranked	1967 citing authors

#	Article	IF	Citations
1	Cytotoxicity and slow release of the anti-cancer drug doxorubicin from ZIF-8. RSC Advances, 2012, 2, 9437.	1.7	247
2	Kinetic and calorimetric study of the adsorption of dyes on mesoporous activated carbon prepared from coconut coir dust. Journal of Colloid and Interface Science, 2006, 298, 515-522.	5.0	151
3	Sparkle model for the quantum chemical AM1 calculation of europium complexes. Chemical Physics Letters, 1994, 227, 349-353.	1.2	128
4	Theoretical and Experimental Studies of the Photoluminescent Properties of the Coordination Polymer [Eu(DPA)(HDPA)(H₂O)₂]Â·4H₂O. Journal of Physical Chemistry B, 2008, 112, 4204-4212.	1.2	81
5	Sparkle Model for AM1 Calculation of Lanthanide Complexes:Â Improved Parameters for Europiumâ€. Inorganic Chemistry, 2004, 43, 2346-2354.	1.9	65
6	Inclusion complexes of pyrimethamine in 2-hydroxypropyl-Î²-cyclodextrin: Characterization, phase solubility and molecular modelling. Bioorganic and Medicinal Chemistry, 2007, 15, 5752-5759.	1.4	56
7	Sulfadiazine/hydroxypropyl-Î²-cyclodextrin hostâ€“guest system: Characterization, phase-solubility and molecular modeling. Bioorganic and Medicinal Chemistry, 2008, 16, 5788-5794.	1.4	54
8	Theoretical and Experimental Spectroscopic Approach of Fluorinated Ln³⁺â^'Î²-Diketonate Complexes. Journal of Physical Chemistry A, 2010, 114, 7928-7936.	1.1	52
9	Sparkle model for the quantum chemical AM1 calculation of europium complexes of coordination number nine. Journal of Alloys and Compounds, 1995, 225, 55-59.	2.8	43
10	Eu(III) and Gd(III) complexes with pirazyne-2-carboxylic acid: luminescence and modelling of the structure and energy transfer process. Journal of Alloys and Compounds, 2004, 366, 124-131.	2.8	41
11	The effect of mechanical grinding on the formation, crystalline changes and dissolution behaviour of the inclusion complex of telmisartan and Î²-cyclodextrins. Carbohydrate Polymers, 2015, 133, 373-383.	5.1	39
12	Sparkle/AM1 Parameters for the Modeling of Samarium(III) and Promethium(III) Complexes. Journal of Chemical Theory and Computation, 2006, 2, 64-74.	2.3	37
13	Design of europium(III) complexes with high quantum yield. Journal of Molecular Modeling, 2005, 12, 16-23.	0.8	36
14	Effect of temperature on formation of two new lanthanide metal-organic frameworks: Synthesis, characterization and theoretical studies of Tm(III)-succinate. Journal of Solid State Chemistry, 2013, 197, 7-13.	1.4	34
15	Sparkle/AM1 Structure Modeling of Lanthanum (III) and Lutetium (III) Complexes. Journal of Physical Chemistry A, 2006, 110, 5897-5900.	1.1	28
16	Sparkle/PM3 Parameters for the Modeling of Neodymium(III), Promethium(III), and Samarium(III) Complexes. Journal of Chemical Theory and Computation, 2007, 3, 1588-1596.	2.3	27
17	Principal Component Analysis of X-ray Diffraction Patterns To Yield Morphological Classification of Brucite Particles. Analytical Chemistry, 2007, 79, 2091-2095.	3.2	27
18	Sparkle model and intensity parameters of the Eu(3-amino-2-carboxypyridine- N -oxide) 3 3H 2 O complex. Computational and Theoretical Chemistry, 2001, 545, 131-135.	1.5	26

#	Article	IF	Citations
19	Synthesis, spectroscopic studies and structure prediction of the new Tb(3-NH2PIC)3Â·3H2O complex. Inorganic Chemistry Communication, 2002, 5, 292-295.	1.8	26
20	Synthesis, sparkle model, intensity parameters and spectroscopic studies of the new Eu(fod) 3 phen-NO complex. Journal of Solid State Chemistry, 2003, 171, 183-188.	1.4	25
21	Are Quantum Chemistry Semiempirical Methods Effective to Predict Solid State Structure and Adsorption in Metal Organic Frameworks?. Journal of Physical Chemistry C, 2015, 119, 23398-23406.	1.5	24
22	Structure Modeling of Trivalent Lanthanum and Lutetium Complexes:â€‰ Sparkle/PM3. Journal of Physical Chemistry A, 2007, 111, 5015-5018.	1.1	23
23	Facile preparation of catalytically active gold nanoparticles on a thiolated chitosan. Materials Letters, 2010, 64, 882-884.	1.3	23
24	Theoretical design of highly luminescent europium (III) complexes: A factorial study. Journal of Photochemistry and Photobiology A: Chemistry, 2011, 217, 389-394.	2.0	22
25	Synthesis, sparkle model and spectroscopic studies of the Eu(hfc)3Â·bipyO2 complex. Journal of Alloys and Compounds, 2004, 374, 320-324.	2.8	21
26	Synthesis, characterization, luminescent properties and theoretical study of two new coordination polymers containing lanthanide [Ce(III) or Yb(III)] and succinate ions. Journal of Molecular Structure, 2013, 1041, 61-67.	1.8	21
27	Excited state calculations of Europium(III) complexes. Journal of Alloys and Compounds, 1997, 250, 412-416.	2.8	20
28	Theoretical Spectroscopic Study of Europium Tris(bipyridine) Cryptates. Journal of Physical Chemistry A, 2012, 116, 4318-4322.	1.1	19
29	The trans effect of lone pairs on individual X-H bonds (X = C or N). An ab initio study. Computational and Theoretical Chemistry, 1994, 305, 19-25.	1.5	18
30	Modeling lanthanide coordination compounds: Sparkle/AM1 parameters for praseodymium (III). Journal of Organometallic Chemistry, 2005, 690, 4099-4102.	0.8	17
31	Characterization, phase solubility and molecular modeling of Î±-cyclodextrin/pyrimethamine inclusion complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 165-170.	2.0	17
32	Would the Pseudocoordination Centre Method Be Appropriate To Describe the Geometries of Lanthanide Complexes?. Journal of Chemical Information and Modeling, 2011, 51, 45-51.	2.5	17
33	Sparkle/AM1 modeling of holmium (III) complexes. Polyhedron, 2005, 24, 3046-3051.	1.0	15
34	Sparkle model for the AM1 calculation of dysprosium (III) complexes. Inorganic Chemistry Communication, 2005, 8, 831-835.	1.8	15
35	Physicochemical study and characterization of the trimethoprim/2-hydroxypropyl-Î³-cyclodextrin inclusion complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 86, 101-106.	2.0	15
36	Host-guest interaction of ZnBDC-MOFÂ+Âdoxorubicin: A theoretical and experimental study. Journal of Molecular Structure, 2017, 1131, 36-42.	1.8	14

#	Article	IF	Citations
37	An IR spectral measure of classical aromaticity in five-and six-membered ring heterocycles: an ab initio study. Computational and Theoretical Chemistry, 1993, 282, 97-104.	1.5	13
38	Uma metodologia para o projeto teÃ³rico de conversores moleculares de luz. Quimica Nova, 1998, 21, 51-59.	0.3	12
39	Spectroscopic properties of the Eu(fod)3Phenâ€“NO incorporated carboxylate glass. Journal of Luminescence, 2006, 116, 132-138.	1.5	12
40	Design of new highly luminescent Tb3+ complexes using theoretical combinatorial chemistry. Journal of Luminescence, 2011, 131, 2487-2491.	1.5	11
41	Interaction of pyrimethamine and sulfadiazine with ionic and neutral micelles: Electronic absorption and fluorescence studies. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2008, 324, 98-104.	2.3	10
42	New experimental and theoretical approach in Eu2O3 microspheres: From synthesis to a study of the energy transfer. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 281, 1-7.	2.0	10
43	Fluorescent tetraruthenated porphyrins embedded in monolithic SiO2 gels by the solâ€“gel process. Journal of Colloid and Interface Science, 2007, 305, 264-269.	5.0	9
44	Structural and theoretical-experimental physicochemical study of trimethoprim/randomly methylated-Î²-cyclodextrin binary system. Carbohydrate Research, 2011, 346, 2746-51.	1.1	9
45	Vibrational spectra and structure of the cis and trans conformers of methyl nitrite: an ab initio MO study. Journal of Molecular Structure, 1996, 375, 153-180.	1.8	8
46	Are the Absorption Spectra of Doxorubicin Properly Described by Considering Different Tautomers?. Journal of Chemical Information and Modeling, 2020, 60, 513-521.	2.5	8
47	Bird's classical aromaticity and ab initio ch intensity parameter in heterocyclic compounds. Journal of Molecular Structure, 1993, 294, 29-31.	1.8	7
48	Theoretical Spectroscopic Study of the Conjugate Microcystin-LR-Europium Cryptate. Journal of the Brazilian Chemical Society, 2013, 24, 236-240.	0.6	7
49	Infrared intensity parameters for furan and thiophene. Computational and Theoretical Chemistry, 1991, 235, 185-188.	1.5	6
50	Sparkle model and photophysical studies of Europium BiqO2-cryptate. Chemical Physics Letters, 2007, 442, 488-491.	1.2	6
51	Improving the quantum efficiency of the lanthanide-organic framework [Eu 2 (MELL)(H 2 O) 6] by heating: A simple strategy to produce efficient luminescent devices. Journal of Luminescence, 2017, 187, 555-563.	1.5	6
52	Host-guest complexes of 2-hydroxypropyl- Î² -cyclodextrin/ Î² -cyclodextrin and nifedipine: 1 H NMR, molecular modeling, and dissolution studies. Journal of Molecular Structure, 2017, 1150, 146-154.	1.8	6
53	Prediction of correct intermolecular interactions in host-guest systems involving cyclodextrins. Journal of Molecular Structure, 2020, 1205, 127517.	1.8	6
54	Would the solvent effect be the main cause of band shift in the theoretical absorption spectrum of large lanthanide complexes?. Journal of Molecular Structure, 2011, 997, 30-36.	1.8	4

#	Article	IF	Citations
55	Lanthanide organic frameworks geometry prediction accuracies of quantum chemical calculations. Journal of Molecular Structure, 2019, 1184, 310-315.	1.8	4
56	Integration of an Inhibitor-like Rule and Structure-based Virtual Screening for the Discovery of Novel Myeloperoxidase Inhibitors. Journal of Chemical Information and Modeling, 2020, 60, 6408-6418.	2.5	2
57	Computer simulation and spectroscopic study of inclusion complexes of cyclodextrins with luminescent porphyrins. Journal of Physics: Conference Series, 2010, 249, 012037.	0.3	1
58	Hydrothermal reactions: From the synthesis of ligand to new lanthanide 3D-coordination polymers. Journal of Solid State Chemistry, 2013, 207, 132-139.	1.4	1