Nivan Bezerra da Costa Junior

List of Publications by Citations

58 papers	1,465 citations	21 h-index	36 g-index
58 ext. papers	1,573 ext. citations	4 avg, IF	3.87 L-index

#	Paper	IF	Citations
58	Cytotoxicity and slow release of the anti-cancer drug doxorubicin from ZIF-8. *RSC Advances*, **2012**, 2, 9437	3.7	193
57	Sparkle model for the quantum chemical AM1 calculation of europium complexes. *Chemical Physics Letters*, **1994**, 227, 349-353	2.5	123
56	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, 515-22	9.3	122
55	Theoretical and experimental studies of the photoluminescent properties of the coordination polymer [Eu(DPA)(HDPA)(H2O)2].4H2O. *Journal of Physical Chemistry B*, **2008**, 112, 4204-12	3.4	81
54	Sparkle model for AM1 calculation of lanthanide complexes: improved parameters for europium. *Inorganic Chemistry*, **2004**, 43, 2346-54	5.1	63
53	Inclusion complexes of pyrimethamine in 2-hydroxypropyl-beta-cyclodextrin: characterization, phase solubility and molecular modelling. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 5752-9	3.4	49
52	Sulfadiazine/hydroxypropyl-beta-cyclodextrin host-guest system: Characterization, phase-solubility and molecular modeling. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 5788-94	3.4	47
51	Theoretical and experimental spectroscopic approach of fluorinated Ln(3+)-beta-diketonate complexes. *Journal of Physical Chemistry A*, **2010**, 114, 7928-36	2.8	46
50	Sparkle model for the quantum chemical AM1 calculation of europium complexes of coordination number nine. *Journal of Alloys and Compounds*, **1995**, 225, 55-59	5.7	43
49	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	5.7	39
48	Design of europium(III) complexes with high quantum yield. *Journal of Molecular Modeling*, **2005**, 12, 16-23	2	35
47	Sparkle/AM1 Parameters for the Modeling of Samarium(III) and Promethium(III) Complexes. *Journal of Chemical Theory and Computation*, **2006**, 2, 64-74	6.4	34
46	The effect of mechanical grinding on the formation, crystalline changes and dissolution behaviour of the inclusion complex of telmisartan and Ecyclodextrins. *Carbohydrate Polymers*, **2015**, 133, 373-83	10.3	26
45	Sparkle/PM3 Parameters for the Modeling of Neodymium(III), Promethium(III), and Samarium(III) Complexes. *Journal of Chemical Theory and Computation*, **2007**, 3, 1588-96	6.4	26
44	Sparkle/AM1 structure modeling of lanthanum (III) and lutetium (III) complexes. *Journal of Physical Chemistry A*, **2006**, 110, 5897-900	2.8	26
43	Synthesis, spectroscopic studies and structure prediction of the new Tb(3-NH2PIC)33H2O complex. *Inorganic Chemistry Communication*, **2002**, 5, 292-295	3.1	26
42	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		26

41	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	3.3	24
40	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	3.3	24
39	Structure modeling of trivalent lanthanum and lutetium complexes: Sparkle/PM3. *Journal of Physical Chemistry A*, **2007**, 111, 5015-8	2.8	22
38	Synthesis, sparkle model and spectroscopic studies of the Eu(hfc)3□bipyO2 complex. *Journal of Alloys and Compounds*, **2004**, 374, 320-324	5.7	21
37	Principal component analysis of X-ray diffraction patterns to yield morphological classification of brucite particles. *Analytical Chemistry*, **2007**, 79, 2091-5	7.8	20
36	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	3.8	19
35	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	3.4	19
34	Excited state calculations of Europium(III) complexes. *Journal of Alloys and Compounds*, **1997**, 250, 412-416	5.7	19
33	Theoretical design of highly luminescent europium (III) complexes: A factorial study. *Journal of Photochemistry and Photobiology A: Chemistry*, **2011**, 217, 389-394	4.7	18
32	Facile preparation of catalytically active gold nanoparticles on a thiolated chitosan. *Materials Letters*, **2010**, 64, 882-884	3.3	18
31	Would the pseudocoordination centre method be appropriate to describe the geometries of lanthanide complexes?. *Journal of Chemical Information and Modeling*, **2011**, 51, 45-51	6.1	17
30	Theoretical spectroscopic study of europium tris(bipyridine) cryptates. *Journal of Physical Chemistry A*, **2012**, 116, 4318-22	2.8	16
29	Modeling lanthanide coordination compounds: Sparkle/AM1 parameters for praseodymium (III). *Journal of Organometallic Chemistry*, **2005**, 690, 4099-4102	2.3	16
28	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		16
27	Sparkle model for the AM1 calculation of dysprosium (III) complexes. *Inorganic Chemistry Communication*, **2005**, 8, 831-835	3.1	15
26	Physicochemical study and characterization of the trimethoprim/2-hydroxypropyl-□-cyclodextrin inclusion complex. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 86, 101-6	4.4	14
25	Characterization, phase solubility and molecular modeling of alpha-cyclodextrin/pyrimethamine inclusion complex. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 72, 165-70	4.4	14
24	Sparkle/AM1 modeling of holmium (III) complexes. *Polyhedron*, **2005**, 24, 3046-3051	2.7	14

23	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		12
22	Uma metodologia para o projeto te□ico de conversores moleculares de luz. *Quimica Nova*, **1998**, 21, 51-59	1.6	11
21	Host-guest interaction of ZnBDC-MOF´+´doxorubicin: A theoretical and experimental study. *Journal of Molecular Structure*, **2017**, 1131, 36-42	3.4	10
20	Spectroscopic properties of the Eu(fod)3Phen□O incorporated carboxylate glass. *Journal of Luminescence*, **2006**, 116, 132-138	3.8	10
19	Fluorescent tetraruthenated porphyrins embedded in monolithic SiO2 gels by the sol-gel process. *Journal of Colloid and Interface Science*, **2007**, 305, 264-9	9.3	9
18	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	4.7	8
17	Structural and theoretical-experimental physicochemical study of trimethoprim/randomly methylated-□-cyclodextrin binary system. *Carbohydrate Research*, **2011**, 346, 2746-51	2.9	8
16	Design of new highly luminescent Tb3+ complexes using theoretical combinatorial chemistry. *Journal of Luminescence*, **2011**, 131, 2487-2491	3.8	8
15	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	5.1	8
14	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	3.4	7
13	Theoretical Spectroscopic Study of the Conjugate Microcystin-LR-Europium Cryptate. *Journal of the Brazilian Chemical Society*, **2013**, 24, 236-240	1.5	7
12	Bird□s classical aromaticity and ab initio ch intensity parameter in heterocyclic compounds. *Journal of Molecular Structure*, **1993**, 294, 29-31	3.4	6
11	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	3.8	5
10	Infrared intensity parameters for furan and thiophene. *Computational and Theoretical Chemistry*, **1991**, 235, 185-188		5
9	Sparkle model and photophysical studies of Europium BiqO2-cryptate. *Chemical Physics Letters*, **2007**, 442, 488-491	2.5	4
8	Host-guest complexes of 2-hydroxypropyl-□-cyclodextrin/□-cyclodextrin and nifedipine: 1H NMR, molecular modeling, and dissolution studies. *Journal of Molecular Structure*, **2017**, 1150, 146-154	3.4	3
7	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	3.4	3
6	Lanthanide organic frameworks geometry prediction accuracies of quantum chemical calculations. *Journal of Molecular Structure*, **2019**, 1184, 310-315	3.4	2

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5	Prediction of correct intermolecular interactions in host-guest systems involving cyclodextrins. *Journal of Molecular Structure*, **2020**, 1205, 127517	3.4	2
4	Are the Absorption Spectra of Doxorubicin Properly Described by Considering Different Tautomers?. *Journal of Chemical Information and Modeling*, **2020**, 60, 513-521	6.1	2
3	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	6.1	2
2	Hydrothermal reactions: From the synthesis of ligand to new lanthanide 3D-coordination polymers. *Journal of Solid State Chemistry*, **2013**, 207, 132-139	3.3	1
1	Computer simulation and spectroscopic study of inclusion complexes of cyclodextrins with luminescent porphyrins. *Journal of Physics: Conference Series*, **2010**, 249, 012037	0.3	1