Alfredo M Simas

List of Publications by Year
in descending order

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114 papers	5,204 citations	147801 31 h-index	91884 69 g-index
115 all docs	115 docs citations	115 times ranked	4072 citing authors

#	Article	IF	Citations
1	NMR and luminescence experiments reveal the structure and symmetry adaptation of a europium ionic liquid to solvent polarity. Dalton Transactions, 2021, 50, 10193-10205.	3.3	3
2	A theorized new class of polyhedral hydrocarbons of molecular formula CnHn and their bottom-up scaffold expansions into hyperstructures. Scientific Reports, 2021, 11, 5576.	3.3	5
3	The complex build algorithm to set up starting structures of lanthanoid complexes with stereochemical control for molecular modeling. Scientific Reports, 2021, 11, 21493.	3.3	2
4	RM1 Semiempirical Model: Chemistry, Pharmaceutical Research, Molecular Biology and Materials Science. Journal of the Brazilian Chemical Society, 2018, , .	0.6	6
5	Stereoisomerism in Lanthanide Complexes: Enumeration, Chirality, Identification, Random Coordination Ratios. Inorganic Chemistry, 2018, 57, 10557-10567.	4.0	8
6	Effects of crystal lattice and counterions on the geometries of metal complexes: Hexaaquomagnesium cation as a case study. Journal of Molecular Structure, 2017, 1134, 458-463.	3.6	0
7	Europium complexes: choice of efficient synthetic routes from RM1 thermodynamic quantities as figures of merit. RSC Advances, 2017, 7, 20811-20823.	3.6	6
8	Europium Complexes: Luminescence Boost by a Single Efficient Antenna Ligand. ACS Omega, 2017, 2, 6786-6794.	3.5	24
9	Chemical Partition of the Radiative Decay Rate of Luminescence of Europium Complexes. Scientific Reports, 2016, 6, 21204.	3.3	24
10	Substantial luminescence enhancement in ternary europium complexes by coordination of different ionic ligands. RSC Advances, 2016, 6, 90934-90943.	3.6	8
11	Synthesis of mixed ligand europium complexes: Verification of predicted luminescence intensification. Journal of Luminescence, 2016, 170, 505-512.	3.1	11
12	Parameters for the RM1 Quantum Chemical Calculation of Complexes of the Trications of Thulium, Ytterbium and Lutetium. PLoS ONE, 2016, 11, e0154500.	2.5	3
13	Europium Luminescence: Electronic Densities and Superdelocalizabilities for a Unique Adjustment of Theoretical Intensity Parameters. Scientific Reports, 2015, 5, 13695.	3.3	33
14	RM1 Semiempirical Quantum Chemistry: Parameters for Trivalent Lanthanum, Cerium and Praseodymium. PLoS ONE, 2015, 10, e0124372.	2.5	5
15	Faster Synthesis of Beta-Diketonate Ternary Europium Complexes: Elapsed Times & Reaction Yields. PLoS ONE, 2015, 10, e0143998.	2.5	10
16	RM1 modeling of neodymium, promethium, and samarium coordination compounds. RSC Advances, 2015, 5, 12403-12408.	3.6	2
17	Semiempirical Quantum Chemistry Model for the Lanthanides: RM1 (Recife Model 1) Parameters for Dysprosium, Holmium and Erbium. PLoS ONE, 2014, 9, e86376.	2.5	10
18	RM1 Model for the Prediction of Geometries of Complexes of the Trications of Eu, Gd, and Tb. Journal of Chemical Theory and Computation, 2014, 10, 3031-3037.	5.3	36

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19	A Comprehensive Strategy to Boost the Quantum Yield of Luminescence of Europium Complexes. Scientific Reports, 2013, 3, 2395.	3.3	101
20	Sparkle/RM1 parameters for the semiempirical quantum chemical calculation of lanthanide complexes. RSC Advances, 2013, 3, 16747.	3.6	58
21	Sparkle/PM7 Lanthanide Parameters for the Modeling of Complexes and Materials. Journal of Chemical Theory and Computation, 2013, 9, 3333-3341.	5.3	107
22	Antinociceptive pyrimidine derivatives: aqueous multicomponent microwave assisted synthesis. Tetrahedron Letters, 2013, 54, 3462-3465.	1.4	29
23	Quantum molecular mechanicsâ€"a noniterative procedure for the fast Ab Initio calculation of closed shell systems. Journal of Computational Chemistry, 2012, 33, 958-969.	3.3	0
24	The lanthanide contraction within the sparkle model. International Journal of Quantum Chemistry, 2011, 111, 1734-1739.	2.0	12
25	Sparkle/PM6 Parameters for all Lanthanide Trications from La(III) to Lu(III). Journal of Chemical Theory and Computation, 2010, 6, 2019-2023.	5.3	84
26	Comparison between the theoretical models and experimental structures of some octacoordinated Ln(III)-bis-dipyridyl-bis-dichloroacetato-diaquo complexes and their phenanthroline analogues. Journal of Rare Earths, 2010, 28, 83-85.	4.8	0
27	Hepatitis C virus infection diagnosis using metabonomics. Journal of Viral Hepatitis, 2010, 17, 854-858.	2.0	47
28	Molecular modeling of the octacoordinated tetracarbonato-Nd(III), [Nd(CO3)4]5â^', complex and its nonacoordinated fluoro- and aquo-adducts. Journal of Rare Earths, 2010, 28, 847-853.	4.8	3
29	1,3-thiazolium-5-thiolates mesoionic compounds: semiempirical evaluation of their first static hyperpolarizabilities and synthesis of new examples. Journal of the Brazilian Chemical Society, 2010, 21, 934-940.	0.6	17
30	Two-Photon Absorption by Fluorene Derivatives: Systematic Molecular Design. Journal of Physical Chemistry C, 2010, 114, 6106-6116.	3.1	21
31	Sparkle/PM3 for the modeling of europium(III), gadolinium(III), and terbium(III) complexes. Journal of the Brazilian Chemical Society, 2009, 20, 1638-1645.	0.6	59
32	Lanthanide coordination compounds modeling: Sparkle/PM3 parameters for dysprosium (III), holmium (III) and erbium (III). Journal of Organometallic Chemistry, 2008, 693, 1952-1956.	1.8	22
33	Two-Photon Absorption Cross-Sections from Electronic Structure Methods: Mesoionic Compounds. Chemistry of Materials, 2008, 20, 4142-4155.	6.7	6
34	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.	5.3	27
35	Structure Modeling of Trivalent Lanthanum and Lutetium Complexes:â€‰ Sparkle/PM3. Journal of Physical Chemistry A, 2007, 111, 5015-5018.	2.5	23
36	Sparkle/PM3 parameters for praseodymium(III) and ytterbium(III). Chemical Physics Letters, 2007, 441, 354-357.	2.6	18

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37	Probing the nuclear susceptibility of mesoionic compounds using two-beam coupling with chirp-controlled pulses. Chemical Physics Letters, 2007, 449, 101-106.	2.6	16
38	Cerium (III) Complexes Modeling with Sparkle/PM3. Lecture Notes in Computer Science, 2007, , 312-318.	1.3	13
39	Sparkle/AM1 Structure Modeling of Lanthanum (III) and Lutetium (III) Complexes. Journal of Physical Chemistry A, 2006, 110, 5897-5900.	2.5	28
40	Photoluminescence of Europium(III) Dithiocarbamate Complexes:â€‰ Electronic Structure, Charge Transfer and Energy Transfer. Journal of Physical Chemistry A, 2006, 110, 2510-2516.	2.5	98
41	Sparkle/AM1 Parameters for the Modeling of Samarium(III) and Promethium(III) Complexes. Journal of Chemical Theory and Computation, 2006, 2, 64-74.	5.3	37
42	B3LYP, RHF and PM5 theoretical studies on phosphorescent cyclometalated Ir(III) complexes. Chemical Physics Letters, 2006, 420, 230-234.	2.6	5
43	Modeling rare earth complexes: Sparkle/PM3 parameters for thulium(III). Chemical Physics Letters, 2006, 425, 138-141.	2.6	36
44	AM1 Sparkle modeling of Er(III) and Ce(III) coordination compounds. Journal of Organometallic Chemistry, 2006, 691, 2584-2588.	1.8	22
45	Sparkle model for AM1 calculation of neodymium(III) coordination compounds. Journal of Photochemistry and Photobiology A: Chemistry, 2006, 177, 225-237.	3.9	23
46	Nonlinear absorption of new mesoionic compounds. Optics Communications, 2006, 264, 225-228.	2.1	19
47	Lanthanide complex coordination polyhedron geometry prediction accuracies of ab initio effective core potential calculations. Journal of Molecular Modeling, 2006, 12, 373-389.	1.8	56
48	RM1: A reparameterization of AM1 for H, C, N, O, P, S, F, Cl, Br, and I. Journal of Computational Chemistry, 2006, 27, 1101-1111.	3.3	634
49	Modeling lanthanide coordination compounds: Sparkle/AM1 parameters for praseodymium (III). Journal of Organometallic Chemistry, 2005, 690, 4099-4102.	1.8	17
50	Efficacy of the semiempirical sparkle model as compared to ECP ab-initio calculations for the prediction of ligand field parameters of europium (III) complexes. Journal of Luminescence, 2005, 111, 81-87.	3.1	32
51	Sparkle/AM1 modeling of holmium (III) complexes. Polyhedron, 2005, 24, 3046-3051.	2.2	15
52	Sparkle model for the AM1 calculation of dysprosium (III) complexes. Inorganic Chemistry Communication, 2005, 8, 831-835.	3.9	15
53	Modeling rare earth complexes: Sparkle/AM1 parameters for thulium (III). Chemical Physics Letters, 2005, 411, 61-65.	2.6	17
54	Modeling lanthanide complexes: Sparkle/AM1 parameters for ytterbium (III). Journal of Computational Chemistry, 2005, 26, 1524-1528.	3.3	18

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55	Theoretical and experimental luminescence quantum yields of coordination compounds of trivalent europium. International Journal of Quantum Chemistry, 2005, 103, 572-579.	2.0	17
56	Theoretical nonlinear optics equivalence between mesoionic and polyenic bridges in push-pull compounds. Journal of the Brazilian Chemical Society, 2005, 16, 583-588.	0.6	11
57	Sparkle Model for the Calculation of Lanthanide Complexes:Â AM1 Parameters for Eu(III), Gd(III), and Tb(III)â€. Inorganic Chemistry, 2005, 44, 3299-3310.	4.0	133
58	Sparkle Model for AM1 Calculation of Lanthanide Complexes:Â Improved Parameters for Europiumâ€. Inorganic Chemistry, 2004, 43, 2346-2354.	4.0	65
59	Synthesis and complete assignments of 1H and 13C NMR spectra of mesoionic 1,3-thiazolium-2 thiolates. Arkivoc, 2004, 2004, 12-21.	0.5	7
60	Efficient Chiral Discrimination by77Se NMR. Organic Letters, 2003, 5, 1601-1604.	4.6	23
61	Synthesis, Characterization and Crystallographic Studies of Three 2-Aryl-3-methyl-4-aryl-1,3-thiazolium-5-thiolates. Synthesis, 2003, 2003, 0685-0690.	2.3	15
62	Self-diffusion of Alkali Ions in Aqueous Solutions of Crown Ether Complexes. Journal of Physical Chemistry A, 2002, 106, 589-594.	2.5	10
63	Synthesis and Characterization of some New Mesoionic 1,3-Thiazolium-5-thiolates via Cyclodehydration and in situ 1,3-Dipolar Cycloaddition/Cycloreversion. Molecules, 2002, 7, 791-800.	3.8	19
64	Reverse saturable absorption and anti-Stokes fluorescence in mesoionic compounds pumped at 532 nm. Applied Optics, 2001, 40, 1389.	2.1	12
65	Diffusion, reaction kinetics and exchange of sodium in aqueous solutions containing a crown ether. Chemical Physics Letters, 2001, 335, 43-49.	2.6	11
66	Ultrafast dynamics of mesoionic liquid solutions studied with incoherent light. Chemical Physics Letters, 2001, 347, 163-166.	2.6	15
67	Exact topological twistons in crystalline polyethylene. Chemical Physics Letters, 2000, 320, 587-593.	2.6	22
68	Two-photon absorption in mesoionic compounds pumped at the visible and at the infrared. Chemical Physics Letters, 2000, 332, 13-18.	2.6	24
69	Spectroscopic properties and design of highly luminescent lanthanide coordination complexes. Coordination Chemistry Reviews, 2000, 196, 165-195.	18.8	1,417
70	Design of ligands to obtain lanthanide ion complexes displaying high quantum efficiencies of luminescence using the sparkle model. Computational and Theoretical Chemistry, 2000, 527, 245-251.	1.5	30
71	Mesoionic Compounds: Amphiphilic Heterocyclic Betaines. Synthesis, 2000, 2000, 1565-1568.	2.3	13
72	SYNTHESIS AND CHARACTERIZATION OF MESOIONIC 1,3,4-TRIAZOLIUM-2-SELENOLATES. Phosphorus, Sulfur and Silicon and the Related Elements, 2000, 161, 115-121.	1.6	6

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73	Synthesis and Antiinflammatory Activity of 3-Aryl-5-Isopropyl-1,2,4-Oxadiazoles. Heterocyclic Communications, 2000, 6, .	1.2	31
74	Importance of Tautomers in the Chemical Behavior of Tetracyclinesâ€. Journal of Pharmaceutical Sciences, 1999, 88, 111-120.	3.3	105
75	Mesoionic rings as third-order non-linear optical materials. Chemical Physics Letters, 1999, 309, 421-426.	2.6	19
76	Synthesis, X-ray Structure, Spectroscopic Characterization, and Theoretical Prediction of the Structure and Electronic Spectrum of Eu(btfa)3Â·bipy and an Assessment of the Effect of Fluorine as a Î²-Diketone Substituent on the Ligandâ^'Metal Energy Transfer Process. Inorganic Chemistry, 1998, 37, 3542-3547.	4.0	113
77	Are mesoionic compounds aromatic?. Canadian Journal of Chemistry, 1998, 76, 869-872.	1.1	26
78	Uma metodologia para o projeto teÃ³rico de conversores moleculares de luz. Quimica Nova, 1998, 21, 51-59.	0.3	12
79	Excited state calculations of Europium(III) complexes. Journal of Alloys and Compounds, 1997, 250, 412-416.	5.5	20
80	Modeling Lanthanide Complexes: Towards the Theoretical Design of Light Conversion Molecular Devices. Molecular Engineering, 1997, 7, 293-308.	0.2	26
81	Synthesis, crystal structure determination and theoretical prediction of the structure and electronic spectrum of Eu(btfa)3bipy. Journal of Luminescence, 1997, 72-74, 159-161.	3.1	19
82	Theoretical model for the prediction of electronic spectra of lanthanide complexes. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 1835-1839.	1.7	58
83	Mesoionic rings as efficient asymmetric bridges for the design of compounds with large optical nonlinearities. Chemical Physics Letters, 1996, 257, 639-646.	2.6	50
84	MESOIONIC 2-N-CYCLOALKYLAMINO-5-ALKYL-1,3-DITHIOLIUM-4-THIOLATES. Phosphorus, Sulfur and Silicon and the Related Elements, 1996, 108, 75-84.	1.6	30
85	Sparkle model for the quantum chemical AM1 calculation of europium complexes of coordination number nine. Journal of Alloys and Compounds, 1995, 225, 55-59.	5.5	43
86	Sparkle model for the quantum chemical AM1 calculation of europium complexes. Chemical Physics Letters, 1994, 227, 349-353.	2.6	128
87	Reaction-fieldâ€“supermolecule approach to calculation of solvent effects. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 189-193.	1.7	34
88	The generator coordinate Hartreeâ€”Fock method for molecular systems. Near Hartreeâ€”Fock limit calculations for N2, CO and BF. Chemical Physics Letters, 1992, 192, 195-198.	2.6	24
89	The generator coordinate Hartree-Fock method for molecular systems. Formalism and first applications to H2, LiH and Li2. Chemical Physics, 1991, 154, 379-384.	1.9	25
90	Infrared intensity parameters for furan and thiophene. Computational and Theoretical Chemistry, 1991, 235, 185-188.	1.5	6

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91	Momentum-space properties of the neutral atoms from H through U. Atomic Data and Nuclear Data Tables, 1991, 48, 213-229.	2.4	17
92	Many-body perturbation theory and coupled-cluster calculations of the ground-state structure of CO3. Chemical Physics Letters, 1991, 177, 98-102.	2.6	14
93	A Gaussian quadrature for the optimal evaluation of integrals involving Lorentzians over a semi-infinite interval. Computer Physics Communications, 1991, 62, 16-24.	7.5	1
94	Generator coordinate gaussian expanded natural orbitals. Computational and Theoretical Chemistry, 1990, 210, 63-70.	1.5	10
95	Topographical features of the Laplacian of the momentum density of atoms and ions most indicative of shell structure. Journal of Chemical Physics, 1989, 90, 6520-6527.	3.0	26
96	The Laplacian of the charge density and its relationship to the shell structure of atoms and ions. Journal of Chemical Physics, 1988, 88, 4367-4374.	3.0	132
97	The quality ofs-orbitals determined by least-squares fitting and constrained variational methods. International Journal of Quantum Chemistry, 1986, 30, 717-735.	2.0	12
98	Electronâ€“nuclear cusp check for self-consistent field wave functions for the neutral atoms from helium to uranium. Canadian Journal of Physics, 1986, 64, 1351-1352.	1.1	10
99	The nonmonotonic behavior of and the presence of slow and fast maxima in the momentum densities of atoms and ions. Journal of Chemical Physics, 1985, 83, 4054-4058.	3.0	45
100	Substituent effects in alkynes and cyanides: a momentum density perspective. Canadian Journal of Chemistry, 1985, 63, 1412-1417.	1.1	12
101	A momentum density analysis of strong hydrogen bonding. Computational and Theoretical Chemistry, 1985, 123, 221-229.	1.5	5
102	Validity of the mass-velocity term in the Breit-Pauli hamiltonian. International Journal of Quantum Chemistry, 1985, 28, 61-68.	2.0	1
103	Relativistic integrals over Breitâ€“Pauli operators. Journal of Chemical Physics, 1984, 81, 5219-5221.	3.0	8
104	The shell structure of atoms and ions in momentum space. Journal of Chemical Physics, 1984, 80, 2636-2642.	3.0	32
105	Partial wave analysis of the momentum density. Journal of Chemical Physics, 1984, 81, 2953-2961.	3.0	27
106	The nodal structure of the momentum distributions of molecules. International Journal of Quantum Chemistry, 1984, 25, 1035-1044.	2.0	10
107	Partial-wave analysis of the momentum densities of 14 electron diatomics. International Journal of Quantum Chemistry, 1984, 26, 385-392.	2.0	15
108	Appraisal of computer hardware and software for quantum-chemical calculations. International Journal of Quantum Chemistry, 1984, 26, 619-638.	2.0	0

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109	Momentum space properties of atoms. International Journal of Quantum Chemistry, 1983, 23, 811-820.	2.0	16
110	Basis set quality. II. Information theoretic appraisal of variouss- orbitals. International Journal of Quantum Chemistry, 1983, 24, 527-550.	2.0	54
111	On the applicability of CNDO indices for the prediction of chemical reactivity. Theoretica Chimica Acta, 1982, 62, 1-16.	0.8	45
112	Momentum space properties of various orbital basis sets used in quantum chemical calculations. International Journal of Quantum Chemistry, 1982, 21, 419-429.	2.0	51
113	Internally folded densities. Chemical Physics, 1981, 63, 175-183.	1.9	69
114	Extraction of momentum expectation values from Compton profiles. Molecular Physics, 1980, 41, 1153-1162.	1.7	42