Ricardo O Freire

List of Publications by Year
in descending order

109	4,245	117571	123376
papers	citations	34 h-index	61 g-index

109	109	109	3841
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	1.5	634
2	Cytotoxicity and slow release of the anti-cancer drug doxorubicin from ZIF-8. RSC Advances, 2012, 2, 9437.	1.7	247
3	LUMPAC lanthanide luminescence software: Efficient and user friendly. Journal of Computational Chemistry, 2014, 35, 772-775.	1.5	184
4	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.	1.9	133
5	Spectroscopic Study of a UV-Photostable Organic-Inorganic Hybrids Incorporating an Eu3+ Î²-Diketonate Complex. ChemPhysChem, 2006, 7, 735-746.	1.0	127
6	3-Phenyl-4-benzoyl-5-isoxazolonate Complex of Eu3+with Tri-n-octylphosphine Oxide as a Promising Light-Conversion Molecular Device. Inorganic Chemistry, 2006, 45, 2184-2192.	1.9	116
7	Sparkle/PM7 Lanthanide Parameters for the Modeling of Complexes and Materials. Journal of Chemical Theory and Computation, 2013, 9, 3333-3341.	2.3	107
8	Tb3+â†'Eu3+ Energy Transfer in Mixed-Lanthanide-Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 19951-19957.	1.5	94
9	Energy Transfer Mechanisms in Organicâ^'Inorganic Hybrids Incorporating Europium(III):â€‰ A Quantitative Assessment by Light Emission Spectroscopy. Journal of Physical Chemistry C, 2007, 111, 17627-17634.	1.5	84
10	Sparkle/PM6 Parameters for all Lanthanide Trications from La(III) to Lu(III). Journal of Chemical Theory and Computation, 2010, 6, 2019-2023.	2.3	84
11	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
12	Tuning of the excitation wavelength from UV to visible region in Eu3+-Î²-diketonate complexes: Comparison of theoretical and experimental photophysical properties. Dalton Transactions, 2011, 40, 3257.	1.6	76
13	Energy Transfer and Emission Quantum Yields of Organicâ^'Inorganic Hybrids Lacking Metal Activator Centers. Journal of Physical Chemistry C, 2007, 111, 3275-3284.	1.5	70
14	A Eu^{III} Tetrakis(Î²-diketonate) Dimeric Complex: Photophysical Properties, Structural Elucidation by Sparkle/AM1 Calculations, and Doping into PMMA Films and Nanowires. Inorganic Chemistry, 2014, 53, 8407-8417.	1.9	67
15	Sparkle Model for AM1 Calculation of Lanthanide Complexes:Â Improved Parameters for Europiumâ€. Inorganic Chemistry, 2004, 43, 2346-2354.	1.9	65
16	Influence of fluorinated chain length on luminescent properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si0094.gif" overflow="scroll"><mml:msup><mml:mrow><mml:mi>Eu</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:math> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si0095.gif" overflow="scroll"><mml:mi>Î²</mml:mi></mml:math>-diketonate complexes. Journal of Luminescence, 2018, 196, 161-168.	1.5	63
17	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
18	Sparkle/RM1 parameters for the semiempirical quantum chemical calculation of lanthanide complexes. RSC Advances, 2013, 3, 16747.	1.7	58

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19	Modeling, Structural, and Spectroscopic Studies of Lanthanide-Organic Frameworks. Journal of Physical Chemistry B, 2009, 113, 12181-12188.	1.2	57
20	Lanthanide complex coordination polyhedron geometry prediction accuracies of ab initio effective core potential calculations. Journal of Molecular Modeling, 2006, 12, 373-389.	0.8	56
21	Synthesis and Characterization of the Europium(III) Pentakis(picrate) Complexes with Imidazolium Countercations: Structural and Photoluminescence Study. Inorganic Chemistry, 2012, 51, 12867-12878.	1.9	54
22	3-Phenyl-4-aroyl-5-isoxazolonate complexes of Tb3+ as promising light-conversion molecular devices. Inorganic Chemistry Communication, 2007, 10, 393-396.	1.8	52
23	Theoretical and Experimental Spectroscopic Approach of Fluorinated Ln³⁺â^Î²-Diketonate Complexes. Journal of Physical Chemistry A, 2010, 114, 7928-7936.	1.1	52
24	Synthesis and Luminescent Properties of Novel Europium(III) Heterocyclic Î²-Diketone Complexes with Lewis Bases: Structural Analysis Using the Sparkle/AM1 Model. European Journal of Inorganic Chemistry, 2005, 2005, 4129-4137.	1.0	47
25	Synthesis, Crystal Structure, and Modelling of a New Tetramer Complex of Europium. Journal of Physical Chemistry B, 2007, 111, 9228-9238.	1.2	44
26	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
27	Theoretical tools for the calculation of the photoluminescent properties of europium systems â€“ A case study. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 256, 29-35.	2.0	41
28	Lanthanide complexes with aromatic o-phosphorylated ligands: synthesis, structure elucidation and photophysical properties. Dalton Transactions, 2014, 43, 3121-3136.	1.6	41
29	New photo/electroluminescent europium(III) Î²-diketonate complex containing a p,pâ€²-disubstituted bipyridine ligand: Synthesis, solid state characterization, theoretical and experimental spectroscopic studies. Inorganica Chimica Acta, 2017, 458, 28-38.	1.2	40
30	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
31	Design of europium(III) complexes with high quantum yield. Journal of Molecular Modeling, 2005, 12, 16-23.	0.8	36
32	Modeling rare earth complexes: Sparkle/PM3 parameters for thulium(III). Chemical Physics Letters, 2006, 425, 138-141.	1.2	36
33	Water-Soluble Tb3+ and Eu3+ Complexes with Ionophilic (Ionically Tagged) Ligands as Fluorescence Imaging Probes. Inorganic Chemistry, 2013, 52, 10199-10205.	1.9	36
34	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.	2.3	36
35	On the use of combinatory chemistry to the design of new luminescent Eu3+ complexes. Chemical Physics Letters, 2005, 405, 123-126.	1.2	35
36	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

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37	Europium Luminescence: Electronic Densities and Superdelocalizabilities for a Unique Adjustment of Theoretical Intensity Parameters. Scientific Reports, 2015, 5, 13695.	1.6	33
38	Synthesis, structural characterization, luminescent properties and theoretical study of three novel lanthanide metal-organic frameworks of Ho(III), Gd(III) and Eu(III) with 2,5-thiophenedicarboxylate anion. Journal of Solid State Chemistry, 2015, 227, 68-78.	1.4	33
39	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.	1.5	32
40	Unusual photoluminescence properties of the 3D mixed-lanthanideâ€“organic frameworks induced by dimeric structures: a theoretical and experimental approach. Physical Chemistry Chemical Physics, 2014, 16, 14858-14866.	1.3	29
41	Sparkle/AM1 Structure Modeling of Lanthanum (III) and Lutetium (III) Complexes. Journal of Physical Chemistry A, 2006, 110, 5897-5900.	1.1	28
42	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
43	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
44	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
45	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
46	Elucidating the energy transfer process in mononuclear and binuclear lanthanide complexes of the anti-inflammatory drug ibuprofen: From synthesis to high luminescence emission. Journal of Luminescence, 2017, 181, 196-210.	1.5	25
47	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
48	Chemical Partition of the Radiative Decay Rate of Luminescence of Europium Complexes. Scientific Reports, 2016, 6, 21204.	1.6	24
49	Sparkle model for AM1 calculation of neodymium(III) coordination compounds. Journal of Photochemistry and Photobiology A: Chemistry, 2006, 177, 225-237.	2.0	23
50	Structure Modeling of Trivalent Lanthanum and Lutetium Complexes:â€‰ Sparkle/PM3. Journal of Physical Chemistry A, 2007, 111, 5015-5018.	1.1	23
51	Bright orange and red light-emitting diodes of new visible light excitable tetrakis-Ln-Î²-diketonate (Ln =) Tj ETQq1 1 0.784314 rgBT /Over	1.4	23
52	Synthesis, characterization and spectroscopic studies of binuclear lanthanide complexes containing the anti-inflammatory drug Ibuprofen and CH3-disubstituted bipyridine ligands: Influence of methyl group position in the photoluminescence. Journal of Luminescence, 2018, 194, 747-759.	1.5	23
53	AM1 Sparkle modeling of Er(III) and Ce(III) coordination compounds. Journal of Organometallic Chemistry, 2006, 691, 2584-2588.	0.8	22
54	Lanthanide coordination compounds modeling: Sparkle/PM3 parameters for dysprosium (III), holmium (III) and erbium (III). Journal of Organometallic Chemistry, 2008, 693, 1952-1956.	0.8	22

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55	New Homotrinuclear Lanthanide Complexes: Synthesis, Characterization and Spectroscopic Study. Journal of Physical Chemistry A, 2010, 114, 10066-10075.	1.1	22
56	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
57	Theoretical and experimental spectroscopic studies of the first highly luminescent binuclear hydrocinnamate of Eu(III), Tb(III) and Gd(III) with bidentate 2,2'-bipyridine ligand. Journal of Luminescence, 2014, 148, 307-316.	1.5	22
58	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
59	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
60	Achieving visible light excitation in carbazole-based Eu³⁺â€“Î²-diketonate complexes via molecular engineering. RSC Advances, 2015, 5, 90720-90730.	1.7	21
61	Tuning the luminescence efficiency by perfluorination of side chains in Eu³⁺ complexes with Î²-diketones of the thiophene series. Physical Chemistry Chemical Physics, 2021, 23, 25748-25760.	1.3	21
62	Modelling the luminescence of extended solids: an example of a highly luminescent MCM-41 impregnated with a Eu³⁺Î²-diketonate complex. Journal of Materials Chemistry C, 2014, 2, 9701-9711.	2.7	20
63	A new Eu(III)/Tb(III) binuclear coordination compound with crown ethers and bridging 4,4â€²-dipyridyl. Journal of Luminescence, 2010, 130, 1946-1951.	1.5	19
64	Theoretical Spectroscopic Study of Europium Tris(bipyridine) Cryptates. Journal of Physical Chemistry A, 2012, 116, 4318-4322.	1.1	19
65	Separation of glycosidic catiomers by TWIMâ€MS using CO₂ as a drift gas. Journal of Mass Spectrometry, 2015, 50, 336-343.	0.7	19
66	Modeling lanthanide complexes: Sparkle/AM1 parameters for ytterbium (III). Journal of Computational Chemistry, 2005, 26, 1524-1528.	1.5	18
67	On the use of theoretical tools in the study of photophysical properties of the new Eu(fod)3 complex with diphenbipy. Chemical Physics Letters, 2006, 418, 337-341.	1.2	18
68	Sparkle/PM3 parameters for praseodymium(III) and ytterbium(III). Chemical Physics Letters, 2007, 441, 354-357.	1.2	18
69	Modeling lanthanide coordination compounds: Sparkle/AM1 parameters for praseodymium (III). Journal of Organometallic Chemistry, 2005, 690, 4099-4102.	0.8	17
70	Modeling rare earth complexes: Sparkle/AM1 parameters for thulium (III). Chemical Physics Letters, 2005, 411, 61-65.	1.2	17
71	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
72	Experimental and Theoretical Studies of Glyphosate Detection in Water by an Europium Luminescent Complex and Effective Adsorption by HKUST-1 and IRMOF-3. Journal of Agricultural and Food Chemistry, 2020, 68, 9664-9672.	2.4	16

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73	New Eu^{III} Pyromellitic Metalâ€“Organic Framework of Intense Red-Orange Luminescence and High Thermal Stability for Marking in Gunshot Residues. Journal of Physical Chemistry C, 2020, 124, 9996-10006.	1.5	16
74	Sparkle/AM1 modeling of holmium (III) complexes. Polyhedron, 2005, 24, 3046-3051.	1.0	15
75	Sparkle model for the AM1 calculation of dysprosium (III) complexes. Inorganic Chemistry Communication, 2005, 8, 831-835.	1.8	15
76	Host-guest interaction of ZnBDC-MOFÂ+Âdoxorubicin: A theoretical and experimental study. Journal of Molecular Structure, 2017, 1131, 36-42.	1.8	14
77	Study of energy transfer mechanism in the EuIII and GdIII homobimetallic complexes containing the anti-inflammatory drug naproxen and N,N-donors ligands. Journal of Luminescence, 2019, 210, 104-118.	1.5	14
78	On the Use of Ligand Field Parameters in the Study of Coordinated Water Molecules in Eu3+Complexes. Journal of Physical Chemistry A, 2005, 109, 4607-4610.	1.1	13
79	Theoretical Methodologies for Calculation of Juddâ€“Ofelt Intensity Parameters of Polyeuropium Systems. Journal of Physical Chemistry A, 2013, 117, 14095-14099.	1.1	13
80	Cerium (III) Complexes Modeling with Sparkle/PM3. Lecture Notes in Computer Science, 2007, , 312-318.	1.0	13
81	Spectroscopic properties of the Eu(fod)3Phenâ€“NO incorporated carboxylate glass. Journal of Luminescence, 2006, 116, 132-138.	1.5	12
82	The lanthanide contraction within the sparkle model. International Journal of Quantum Chemistry, 2011, 111, 1734-1739.	1.0	12
83	Mononuclear lanthanide(<scp>iii</scp>)-oxamate complexes as new photoluminescent field-induced single-molecule magnets: solid-state photophysical and magnetic properties. Dalton Transactions, 2020, 49, 16106-16124.	1.6	12
84	Design of new highly luminescent Tb3+ complexes using theoretical combinatorial chemistry. Journal of Luminescence, 2011, 131, 2487-2491.	1.5	11
85	Semiempirical Quantum Chemistry Model for the Lanthanides: RM1 (Recife Model 1) Parameters for Dysprosium, Holmium and Erbium. PLoS ONE, 2014, 9, e86376.	1.1	10
86	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
87	Equilibrium states and zero temperature limit on topologically transitive countable Markov shifts. Transactions of the American Mathematical Society, 2018, 370, 8451-8465.	0.5	10
88	Synthesis, modeling of the structure and kinetic study of the thermal decomposition of La(III) and Nd(III) complexes with 3-hydroxypicolinic acid. Journal of Non-Crystalline Solids, 2005, 351, 394-400.	1.5	9
89	Estudos espectroscÃ³picos e estruturais dos polÃmeros de coordenaÃ§Ã£o 2D, âˆž[Tb(DPA)(HDPA)] e âˆž[Gd(DPA)(HDPA)]. Quimica Nova, 2009, 32, 286-291.	0.3	8
90	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

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91	Structure elucidation of lanthanide complexes by theoretical tools. Chemical Physics Letters, 2007, 443, 378-382.	1.2	7
92	Lanthanide Contraction in Lanthanide Organic Frameworks: A Theoretical and Experimental Study. Journal of Physical Chemistry A, 2020, 124, 7678-7684.	1.1	7
93	Theoretical Spectroscopic Study of the Conjugate Microcystin-LR-Europium Cryptate. Journal of the Brazilian Chemical Society, 2013, 24, 236-240.	0.6	7
94	Sparkle model and photophysical studies of Europium BiqO2-cryptate. Chemical Physics Letters, 2007, 442, 488-491.	1.2	6
95	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
96	RM1 Semiempirical Model: Chemistry, Pharmaceutical Research, Molecular Biology and Materials Science. Journal of the Brazilian Chemical Society, 2018, , .	0.6	6
97	Prediction of correct intermolecular interactions in host-guest systems involving cyclodextrins. Journal of Molecular Structure, 2020, 1205, 127517.	1.8	6
98	IRMOF â€8: Theoretical evaluation of aluminum doping on hydrogen, methane, and hydrogen sulfide adsorption. International Journal of Quantum Chemistry, 2021, 121, e26510.	1.0	6
99	B3LYP, RHF and PM5 theoretical studies on phosphorescent cyclometalated Ir(III) complexes. Chemical Physics Letters, 2006, 420, 230-234.	1.2	5
100	RM1 Semiempirical Quantum Chemistry: Parameters for Trivalent Lanthanum, Cerium and Praseodymium. PLoS ONE, 2015, 10, e0124372.	1.1	5
101	Estimating the Individual Spectroscopic Properties of Three Unique Eu^{III} Sites in a Coordination Polymer. Inorganic Chemistry, 2018, 57, 15421-15429.	1.9	5
102	A relation between the structural diversity and photoluminescent properties in three new classes of Eu3+ hydrocinnamate complexes containing N,N-bidentate and N,N,N-tridentate ancillary ligands. Journal of Luminescence, 2021, 239, 118398.	1.5	5
103	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
104	Lanthanide organic frameworks geometry prediction accuracies of quantum chemical calculations. Journal of Molecular Structure, 2019, 1184, 310-315.	1.8	4
105	Experimental and theoretical study of isoreticular lanthanoid organic framework (LOF): Structure and luminescence. Journal of Luminescence, 2020, 223, 117179.	1.5	4
106	Parameters for the RM1 Quantum Chemical Calculation of Complexes of the Trications of Thulium, Ytterbium and Lutetium. PLoS ONE, 2016, 11, e0154500.	1.1	3
107	RM1 modeling of neodymium, promethium, and samarium coordination compounds. RSC Advances, 2015, 5, 12403-12408.	1.7	2
108	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

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109	Photoluminescent complexes of Eu(III), Tb(III) and Gd(III) with 3-thiopheneacetate and 4,4â€²-dimethyl-2,2â€²-bipyridine: Synthesis, characterization and photophysical properties. Journal of Luminescence, 2022, , 118990.	1.5	1