

Ricardo O Freire

List of Publications by Year in descending order

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109
papers

4,245
citations

117571

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h-index

123376

61
g-index

109
all docs

109
docs citations

109
times ranked

3841
citing authors

#	ARTICLE	IF	CITATIONS
1	Photoluminescent complexes of Eu(III), Tb(III) and Gd(III) with 3-thiopheneacetate and 4,4'-dimethyl-2,2'-bipyridine: Synthesis, characterization and photophysical properties. <i>Journal of Luminescence</i> , 2022, , 118990.	1.5	1
2	IRMOF-8: Theoretical evaluation of aluminum doping on hydrogen, methane, and hydrogen sulfide adsorption. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26510.	1.0	6
3	A relation between the structural diversity and photoluminescent properties in three new classes of Eu ³⁺ hydrocinnamate complexes containing N,N-bidentate and N,N,N-tridentate ancillary ligands. <i>Journal of Luminescence</i> , 2021, 239, 118398.	1.5	5
4	Tuning the luminescence efficiency by perfluorination of side chains in Eu ³⁺ complexes with 1 ² -diketones of the thiophene series. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25748-25760.	1.3	21
5	Prediction of correct intermolecular interactions in host-guest systems involving cyclodextrins. <i>Journal of Molecular Structure</i> , 2020, 1205, 127517.	1.8	6
6	Are the Absorption Spectra of Doxorubicin Properly Described by Considering Different Tautomers?. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 513-521.	2.5	8
7	Lanthanide Contraction in Lanthanide Organic Frameworks: A Theoretical and Experimental Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7678-7684.	1.1	7
8	Mononuclear lanthanide(III)-oxamate complexes as new photoluminescent field-induced single-molecule magnets: solid-state photophysical and magnetic properties. <i>Dalton Transactions</i> , 2020, 49, 16106-16124.	1.6	12
9	Experimental and Theoretical Studies of Glyphosate Detection in Water by an Europium Luminescent Complex and Effective Adsorption by HKUST-1 and IRMOF-3. <i>Journal of Agricultural and Food Chemistry</i> , 2020, 68, 9664-9672.	2.4	16
10	Experimental and theoretical study of isorecticular lanthanoid organic framework (LOF): Structure and luminescence. <i>Journal of Luminescence</i> , 2020, 223, 117179.	1.5	4
11	New Eu ^{III} Pyromellitic Metal-Organic Framework of Intense Red-Orange Luminescence and High Thermal Stability for Marking in Gunshot Residues. <i>Journal of Physical Chemistry C</i> , 2020, 124, 9996-10006.	1.5	16
12	Lanthanide organic frameworks geometry prediction accuracies of quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2019, 1184, 310-315.	1.8	4
13	Study of energy transfer mechanism in the Eu(III) and Gd(III) homobimetallic complexes containing the anti-inflammatory drug naproxen and N,N-donors ligands. <i>Journal of Luminescence</i> , 2019, 210, 104-118.	1.5	14
14	Synthesis, characterization and spectroscopic studies of binuclear lanthanide complexes containing the anti-inflammatory drug ibuprofen and CH ₃ -disubstituted bipyridine ligands: Influence of methyl group position in the photoluminescence. <i>Journal of Luminescence</i> , 2018, 194, 747-759.	1.5	23
15	Photoluminescent complexes of Eu(III), Tb(III) and Gd(III) with 3-thiopheneacetate and 4,4'-dimethyl-2,2'-bipyridine: Synthesis, characterization and photophysical properties. <i>Journal of Luminescence</i> , 2018, 196, 161-168.	1.5	63
16	RM1 Semiempirical Model: Chemistry, Pharmaceutical Research, Molecular Biology and Materials Science. <i>Journal of the Brazilian Chemical Society</i> , 2018, , .	0.6	6
17	Estimating the Individual Spectroscopic Properties of Three Unique Eu ^{III} Sites in a Coordination Polymer. <i>Inorganic Chemistry</i> , 2018, 57, 15421-15429.	1.9	5
18	Equilibrium states and zero temperature limit on topologically transitive countable Markov shifts. <i>Transactions of the American Mathematical Society</i> , 2018, 370, 8451-8465.	0.5	10

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19	Bright orange and red light-emitting diodes of new visible light excitable tetrakis-Ln- β^2 -diketonate (Ln =) Tj ETQq1 1,0,784314,rgBT /Ome	1.4	23
20	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. <i>Journal of Luminescence</i> , 2017, 187, 555-563.	1.5	6
21	New photo/electroluminescent europium(III) β^2 -diketonate complex containing a p,p'-disubstituted bipyridine ligand: Synthesis, solid state characterization, theoretical and experimental spectroscopic studies. <i>Inorganica Chimica Acta</i> , 2017, 458, 28-38.	1.2	40
22	Host-guest interaction of ZnBDC-MOF + Doxorubicin: A theoretical and experimental study. <i>Journal of Molecular Structure</i> , 2017, 1131, 36-42.	1.8	14
23	Elucidating the energy transfer process in mononuclear and binuclear lanthanide complexes of the anti-inflammatory drug ibuprofen: From synthesis to high luminescence emission. <i>Journal of Luminescence</i> , 2017, 181, 196-210.	1.5	25
24	Chemical Partition of the Radiative Decay Rate of Luminescence of Europium Complexes. <i>Scientific Reports</i> , 2016, 6, 21204.	1.6	24
25	Parameters for the RM1 Quantum Chemical Calculation of Complexes of the Trications of Thulium, Ytterbium and Lutetium. <i>PLoS ONE</i> , 2016, 11, e0154500.	1.1	3
26	Europium Luminescence: Electronic Densities and Superdelocalizabilities for a Unique Adjustment of Theoretical Intensity Parameters. <i>Scientific Reports</i> , 2015, 5, 13695.	1.6	33
27	Separation of glycosidic cationomers by TWIM-MS using CO ₂ as a drift gas. <i>Journal of Mass Spectrometry</i> , 2015, 50, 336-343.	0.7	19
28	RM1 Semiempirical Quantum Chemistry: Parameters for Trivalent Lanthanum, Cerium and Praseodymium. <i>PLoS ONE</i> , 2015, 10, e0124372.	1.1	5
29	RM1 modeling of neodymium, promethium, and samarium coordination compounds. <i>RSC Advances</i> , 2015, 5, 12403-12408.	1.7	2
30	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. <i>Journal of Solid State Chemistry</i> , 2015, 227, 68-78.	1.4	33
31	Are Quantum Chemistry Semiempirical Methods Effective to Predict Solid State Structure and Adsorption in Metal Organic Frameworks?. <i>Journal of Physical Chemistry C</i> , 2015, 119, 23398-23406.	1.5	24
32	Achieving visible light excitation in carbazole-based Eu ³⁺ - β^2 -diketonate complexes via molecular engineering. <i>RSC Advances</i> , 2015, 5, 90720-90730.	1.7	21
33	Semiempirical Quantum Chemistry Model for the Lanthanides: RM1 (Recife Model 1) Parameters for Dysprosium, Holmium and Erbium. <i>PLoS ONE</i> , 2014, 9, e86376.	1.1	10
34	Modelling the luminescence of extended solids: an example of a highly luminescent MCM-41 impregnated with a Eu ³⁺ - β^2 -diketonate complex. <i>Journal of Materials Chemistry C</i> , 2014, 2, 9701-9711.	2.7	20
35	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. <i>Journal of Luminescence</i> , 2014, 148, 307-316.	1.5	22
36	New experimental and theoretical approach in Eu ₂ O ₃ microspheres: From synthesis to a study of the energy transfer. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2014, 281, 1-7.	2.0	10

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37	Lanthanide complexes with aromatic o-phosphorylated ligands: synthesis, structure elucidation and photophysical properties. Dalton Transactions, 2014, 43, 3121-3136.	1.6	41
38	A Eu ^{III} Tetrakis(<i>l</i> ² -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
39	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
40	Unusual photoluminescence properties of the 3D mixed-lanthanide-organic frameworks induced by dimeric structures: a theoretical and experimental approach. Physical Chemistry Chemical Physics, 2014, 16, 14858-14866.	1.3	29
41	LUMPAC lanthanide luminescence software: Efficient and user friendly. Journal of Computational Chemistry, 2014, 35, 772-775.	1.5	184
42	Water-Soluble Tb ³⁺ and Eu ³⁺ Complexes with Ionophilic (Ionically Tagged) Ligands as Fluorescence Imaging Probes. Inorganic Chemistry, 2013, 52, 10199-10205.	1.9	36
43	Sparkle/RM1 parameters for the semiempirical quantum chemical calculation of lanthanide complexes. RSC Advances, 2013, 3, 16747.	1.7	58
44	Theoretical Methodologies for Calculation of Judd-Ofelt Intensity Parameters of Polyeuropium Systems. Journal of Physical Chemistry A, 2013, 117, 14095-14099.	1.1	13
45	Sparkle/PM7 Lanthanide Parameters for the Modeling of Complexes and Materials. Journal of Chemical Theory and Computation, 2013, 9, 3333-3341.	2.3	107
46	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
47	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
48	Theoretical tools for the calculation of the photoluminescent properties of europium systems – A case study. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 256, 29-35.	2.0	41
49	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
50	Theoretical Spectroscopic Study of the Conjugate Microcystin-LR-Europium Cryptate. Journal of the Brazilian Chemical Society, 2013, 24, 236-240.	0.6	7
51	Tb ³⁺ +Eu ³⁺ Energy Transfer in Mixed-Lanthanide-Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 19951-19957.	1.5	94
52	Cytotoxicity and slow release of the anti-cancer drug doxorubicin from ZIF-8. RSC Advances, 2012, 2, 9437.	1.7	247
53	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
54	Theoretical Spectroscopic Study of Europium Tris(bipyridine) Cryptates. Journal of Physical Chemistry A, 2012, 116, 4318-4322.	1.1	19

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55	Would the Pseudocoordination Centre Method Be Appropriate To Describe the Geometries of Lanthanide Complexes?. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 45-51.	2.5	17
56	Tuning of the excitation wavelength from UV to visible region in Eu ³⁺ -diketonate complexes: Comparison of theoretical and experimental photophysical properties. <i>Dalton Transactions</i> , 2011, 40, 3257.	1.6	76
57	The lanthanide contraction within the sparkle model. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1734-1739.	1.0	12
58	Would the solvent effect be the main cause of band shift in the theoretical absorption spectrum of large lanthanide complexes?. <i>Journal of Molecular Structure</i> , 2011, 997, 30-36.	1.8	4
59	Theoretical design of highly luminescent europium (III) complexes: A factorial study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2011, 217, 389-394.	2.0	22
60	Design of new highly luminescent Tb ³⁺ complexes using theoretical combinatorial chemistry. <i>Journal of Luminescence</i> , 2011, 131, 2487-2491.	1.5	11
61	Sparkle/PM6 Parameters for all Lanthanide Trications from La(III) to Lu(III). <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2019-2023.	2.3	84
62	Theoretical and Experimental Spectroscopic Approach of Fluorinated Ln ³⁺ -Diketonate Complexes. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7928-7936.	1.1	52
63	A new Eu(III)/Tb(III) binuclear coordination compound with crown ethers and bridging 4,4'-dipyridyl. <i>Journal of Luminescence</i> , 2010, 130, 1946-1951.	1.5	19
64	New Homotrinnuclear Lanthanide Complexes: Synthesis, Characterization and Spectroscopic Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10066-10075.	1.1	22
65	Estudos espectroscópicos e estruturais dos polímeros de coordenação 2D, [Tb(DPA)(HDPA)] e [Gd(DPA)(HDPA)]. <i>Química Nova</i> , 2009, 32, 286-291.	0.3	8
66	Sparkle/PM3 for the modeling of europium(III), gadolinium(III), and terbium(III) complexes. <i>Journal of the Brazilian Chemical Society</i> , 2009, 20, 1638-1645.	0.6	59
67	Modeling, Structural, and Spectroscopic Studies of Lanthanide-Organic Frameworks. <i>Journal of Physical Chemistry B</i> , 2009, 113, 12181-12188.	1.2	57
68	Lanthanide coordination compounds modeling: Sparkle/PM3 parameters for dysprosium (III), holmium (III) and erbium (III). <i>Journal of Organometallic Chemistry</i> , 2008, 693, 1952-1956.	0.8	22
69	Theoretical and Experimental Studies of the Photoluminescent Properties of the Coordination Polymer [Eu(DPA)(HDPA)(H ₂ O) ₂] ₂ ·4H ₂ O. <i>Journal of Physical Chemistry B</i> , 2008, 112, 4204-4212.	1.2	81
70	Sparkle/PM3 Parameters for the Modeling of Neodymium(III), Promethium(III), and Samarium(III) Complexes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1588-1596.	2.3	27
71	Structure Modeling of Trivalent Lanthanum and Lutetium Complexes: Sparkle/PM3. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5015-5018.	1.1	23
72	Energy Transfer Mechanisms in Organic-Inorganic Hybrids Incorporating Europium(III): A Quantitative Assessment by Light Emission Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2007, 111, 17627-17634.	1.5	84

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73	Energy Transfer and Emission Quantum Yields of Organic-Inorganic Hybrids Lacking Metal Activator Centers. <i>Journal of Physical Chemistry C</i> , 2007, 111, 3275-3284.	1.5	70
74	Sparkle/PM3 parameters for praseodymium(III) and ytterbium(III). <i>Chemical Physics Letters</i> , 2007, 441, 354-357.	1.2	18
75	Sparkle model and photophysical studies of Europium BqO ₂ -cryptate. <i>Chemical Physics Letters</i> , 2007, 442, 488-491.	1.2	6
76	Structure elucidation of lanthanide complexes by theoretical tools. <i>Chemical Physics Letters</i> , 2007, 443, 378-382.	1.2	7
77	3-Phenyl-4-aryl-5-isoxazonate complexes of Tb ³⁺ as promising light-conversion molecular devices. <i>Inorganic Chemistry Communication</i> , 2007, 10, 393-396.	1.8	52
78	Synthesis, Crystal Structure, and Modelling of a New Tetramer Complex of Europium. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9228-9238.	1.2	44
79	Cerium (III) Complexes Modeling with Sparkle/PM3. <i>Lecture Notes in Computer Science</i> , 2007, , 312-318.	1.0	13
80	Sparkle/AM1 Structure Modeling of Lanthanum (III) and Lutetium (III) Complexes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5897-5900.	1.1	28
81	Sparkle/AM1 Parameters for the Modeling of Samarium(III) and Promethium(III) Complexes. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 64-74.	2.3	37
82	On the use of theoretical tools in the study of photophysical properties of the new Eu(fod) ₃ complex with diphenbipy. <i>Chemical Physics Letters</i> , 2006, 418, 337-341.	1.2	18
83	B3LYP, RHF and PM5 theoretical studies on phosphorescent cyclometalated Ir(III) complexes. <i>Chemical Physics Letters</i> , 2006, 420, 230-234.	1.2	5
84	Modeling rare earth complexes: Sparkle/PM3 parameters for thulium(III). <i>Chemical Physics Letters</i> , 2006, 425, 138-141.	1.2	36
85	AM1 Sparkle modeling of Er(III) and Ce(III) coordination compounds. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 2584-2588.	0.8	22
86	Sparkle model for AM1 calculation of neodymium(III) coordination compounds. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2006, 177, 225-237.	2.0	23
87	Spectroscopic properties of the Eu(fod) ₃ Phen-NO incorporated carboxylate glass. <i>Journal of Luminescence</i> , 2006, 116, 132-138.	1.5	12
88	3-Phenyl-4-benzoyl-5-isoxazonate Complex of Eu ³⁺ with Tri-n-octylphosphine Oxide as a Promising Light-Conversion Molecular Device. <i>Inorganic Chemistry</i> , 2006, 45, 2184-2192.	1.9	116
89	Lanthanide complex coordination polyhedron geometry prediction accuracies of ab initio effective core potential calculations. <i>Journal of Molecular Modeling</i> , 2006, 12, 373-389.	0.8	56
90	RM1: A reparameterization of AM1 for H, C, N, O, P, S, F, Cl, Br, and I. <i>Journal of Computational Chemistry</i> , 2006, 27, 1101-1111.	1.5	634

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91	Spectroscopic Study of a UV-Photostable Organic-Inorganic Hybrids Incorporating an Eu ³⁺ β^2 -Diketonate Complex. <i>ChemPhysChem</i> , 2006, 7, 735-746.	1.0	127
92	Modeling lanthanide coordination compounds: Sparkle/AM1 parameters for praseodymium (III). <i>Journal of Organometallic Chemistry</i> , 2005, 690, 4099-4102.	0.8	17
93	Efficacy of the semiempirical sparkle model as compared to ECP ab-initio calculations for the prediction of ligand field parameters of europium (III) complexes. <i>Journal of Luminescence</i> , 2005, 111, 81-87.	1.5	32
94	Sparkle/AM1 modeling of holmium (III) complexes. <i>Polyhedron</i> , 2005, 24, 3046-3051.	1.0	15
95	Sparkle model for the AM1 calculation of dysprosium (III) complexes. <i>Inorganic Chemistry Communication</i> , 2005, 8, 831-835.	1.8	15
96	On the use of combinatory chemistry to the design of new luminescent Eu ³⁺ complexes. <i>Chemical Physics Letters</i> , 2005, 405, 123-126.	1.2	35
97	Modeling rare earth complexes: Sparkle/AM1 parameters for thulium (III). <i>Chemical Physics Letters</i> , 2005, 411, 61-65.	1.2	17
98	Modeling lanthanide complexes: Sparkle/AM1 parameters for ytterbium (III). <i>Journal of Computational Chemistry</i> , 2005, 26, 1524-1528.	1.5	18
99	Synthesis and Luminescent Properties of Novel Europium(III) Heterocyclic β^2 -Diketone Complexes with Lewis Bases: Structural Analysis Using the Sparkle/AM1 Model. <i>European Journal of Inorganic Chemistry</i> , 2005, 2005, 4129-4137.	1.0	47
100	Design of europium(III) complexes with high quantum yield. <i>Journal of Molecular Modeling</i> , 2005, 12, 16-23.	0.8	36
101	Sparkle Model for the Calculation of Lanthanide Complexes: AM1 Parameters for Eu(III), Gd(III), and Tb(III). <i>Inorganic Chemistry</i> , 2005, 44, 3299-3310.	1.9	133
102	On the Use of Ligand Field Parameters in the Study of Coordinated Water Molecules in Eu ³⁺ Complexes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4607-4610.	1.1	13
103	Synthesis, modeling of the structure and kinetic study of the thermal decomposition of La(III) and Nd(III) complexes with 3-hydroxypicolinic acid. <i>Journal of Non-Crystalline Solids</i> , 2005, 351, 394-400.	1.5	9
104	Sparkle Model for AM1 Calculation of Lanthanide Complexes: Improved Parameters for Europium. <i>Inorganic Chemistry</i> , 2004, 43, 2346-2354.	1.9	65
105	Synthesis, sparkle model and spectroscopic studies of the Eu(hfc) ₃ -bipyO ₂ complex. <i>Journal of Alloys and Compounds</i> , 2004, 374, 320-324.	2.8	21
106	Eu(III) and Gd(III) complexes with pirazyn-2-carboxylic acid: luminescence and modelling of the structure and energy transfer process. <i>Journal of Alloys and Compounds</i> , 2004, 366, 124-131.	2.8	41
107	Synthesis, sparkle model, intensity parameters and spectroscopic studies of the new Eu(fod) ₃ phen-NO complex. <i>Journal of Solid State Chemistry</i> , 2003, 171, 183-188.	1.4	25
108	Synthesis, spectroscopic studies and structure prediction of the new Tb(3-NH ₂ PIC) ₃ ·3H ₂ O complex. <i>Inorganic Chemistry Communication</i> , 2002, 5, 292-295.	1.8	26

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109	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