Paulo J Costa

List of Publications by Year in descending order

82 papers	2,763 citations	172457 29 h-index	182427 51 g-index
105 all docs	105 docs citations	105 times ranked	3215 citing authors

#	Article	IF	Citations
1	Fluorescent Charge-Assisted Halogen-Bonding Macrocyclic Halo-Imidazolium Receptors for Anion Recognition and Sensing in Aqueous Media. Journal of the American Chemical Society, 2012, 134, 11533-11541.	13.7	199
2	A Halogenâ€Bonding Catenane for Anion Recognition and Sensing. Angewandte Chemie - International Edition, 2012, 51, 1876-1880.	13.8	190
3	Halogen Bond Anion Templated Assembly of an Imidazolium Pseudorotaxane. Angewandte Chemie - International Edition, 2010, 49, 5322-5326.	13.8	147
4	Chloride, carboxylate and carbonate transport by ortho-phenylenediamine-based bisureas. Chemical Science, 2013, 4, 103-117.	7.4	119
5	Towards predictable transmembrane transport: QSAR analysis of anion binding and transport. Chemical Science, 2013, 4, 3036.	7.4	104
6	Structural Studies on Dinuclear Ruthenium(II) Complexes That Bind Diastereoselectively to an Antiparallel Folded Human Telomere Sequence. Journal of Medicinal Chemistry, 2013, 56, 8674-8683.	6.4	103
7	Olefin epoxidation with tert-butyl hydroperoxide catalyzed by MoO2X2L complexes: a DFT mechanistic study. Dalton Transactions, 2006, , 1383.	3.3	88
8	Sulfate anion templated synthesis of a triply interlocked capsule. Chemical Communications, 2009, , 7134.	4.1	88
9	Olefin Epoxidation Catalyzed by Î·⁵-Cyclopentadienyl Molybdenum Compounds: A Computational Study. Organometallics, 2010, 29, 303-311.	2.3	84
10	A Catenane Assembled through a Single Chargeâ€Assisted Halogen Bond. Angewandte Chemie - International Edition, 2013, 52, 4356-4360.	13.8	83
11	Hydrogen activation by high-valent oxo-molybdenum(vi) and -rhenium(vii) and -(v) compounds. Dalton Transactions, 2008, , 1727.	3.3	80
12	MoO₂Cl₂ as a Novel Catalyst for Câ^'P Bond Formation and for Hydrophosphonylation of Aldehydes. Organometallics, 2009, 28, 6206-6212.	2.3	74
13	Catalyzing Aldehyde Hydrosilylation with a Molybdenum(VI) Complex: A Density Functional Theory Study. Chemistry - A European Journal, 2007, 13, 3934-3941.	3.3	72
14	[Re(Î·5-C5H5)(CO)3]+Family of 17-Electron Compounds:Â Monomer/Dimer Equilibria and Other Reactions. Journal of the American Chemical Society, 2008, 130, 2692-2703.	13.7	69
15	Formation of pyridine from acetylenes and nitriles catalyzed by RuCpCl, CoCp, and RhCp derivatives â€“ A computational mechanistic study. Journal of Organometallic Chemistry, 2006, 691, 4434-4445.	1.8	62
16	Synthesis, Structural Characterization, and Theoretical Studies of Gold(I) and Gold(I)â^'Gold(III) Thiolate Complexes:Â Quenching of Gold(I) Thiolate Luminescence. Inorganic Chemistry, 2006, 45, 1059-1068.	4.0	61
17	Rotaxanes Capable of Recognising Chloride in Aqueous Media. Chemistry - A European Journal, 2010, 16, 13082-13094.	3.3	61
18	Electrochemical Oxidation of CoCp(CO)2:Â Radicalâ^'Substrate Reaction of a 17 e-/18 e-Pair and Production of a Unique Dimer Radical. Journal of the American Chemical Society, 2006, 128, 16587-16599.	13.7	57

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19	Tunable transmembrane chloride transport by bis-indolylureas. Chemical Science, 2012, 3, 1436.	7.4	53
20	CNN Pincer Ruthenium Catalysts for Hydrogenation and Transfer Hydrogenation of Ketones: Experimental and Computational Studies. Chemistry - A European Journal, 2014, 20, 13603-13617.	3.3	47
21	New copper(I) and heteronuclear copper(I)â€“ruthenium(II) complexes: Synthesis, structural characterization and cytotoxicity. Journal of Inorganic Biochemistry, 2017, 169, 68-78.	3.5	39
22	The halogen bond: Nature and applications. ChemistrySelect, 2017, 2, .	1.5	39
23	Halogen bonding in halocarbon-protein complexes and computational tools for rational drug design. Expert Opinion on Drug Discovery, 2019, 14, 805-820.	5.0	36
24	Anodic Preparation of [Re2Cp2(CO)6]2+:Â A Dimeric Dication that Provides the Powerful One-Electron Oxidant [ReCp(CO)3]+. Journal of the American Chemical Society, 2005, 127, 15676-15677.	13.7	34
25	Halogen Bonding: An Underestimated Player in Membraneâ€“Ligand Interactions. Journal of the American Chemical Society, 2021, 143, 4253-4267.	13.7	34
26	Group 11 complexes with the bis(3,5-dimethylpyrazol-1-yl)methane ligand. How secondary bonds can influence the coordination environment of Ag(i): the role of coordinated water in [Ag2(Âµ-L)2(OH2)2](OTf)2. Dalton Transactions, 2006, , 4104-4113.	3.3	33
27	Expanding the role of oxo-molybdenum(vi) catalysts: a DFT interpretation of Xâ€“H activation leading to reduction or oxidation. Dalton Transactions, 2009, , 8155.	3.3	33
28	Investigating the Imidazoliumâ€“Anion Interaction through the Anionâ€Templated Construction of Interpenetrated and Interlocked Assemblies. Chemistry - A European Journal, 2011, 17, 12955-12966.	3.3	30
29	Unveiling the Mechanisms of Catalytic Oxidation Reactions Mediated by Oxo-Molybdenum Complexes: A Computational Overview. Current Organic Chemistry, 2012, 16, 65-72.	1.6	26
30	N-Salicylideneamino acidato complexes of oxovanadium(iv). The cysteine and penicillamine complexes. Dalton Transactions, 2004, , 2855.	3.3	24
31	Charge Parametrization of the DvH-c₃ Heme Group: Validation Using Constant-(pH,E) Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 70-82.	2.6	24
32	New [(Î·⁵-C₅H₅)Ru(Nâ€“N)(PPh₃)][PF₆] compounds: colon anticancer activity and GLUT-mediated cellular uptake of carbohydrate-appended complexes. Dalton Transactions, 2016, 45, 11926-11930.	3.3	23
33	Benzene and heterocyclic rings formation in cycloaddition reactions catalyzed by RuCp derivatives: DFT studies. Inorganica Chimica Acta, 2011, 374, 24-35.	2.4	21
34	Synthesis and Theoretical Studies of a Double Helical Complex with the Ligand 4â€²,4â€²â€²-Bis(ferrocenyl)-2,2â€²:6â€²,2â€²â€²:6â€²,2â€²â€²â€²:6â€²â€²,2â€²â€²â€²â€²-quinquepyridine. European Jo 2004, 3038-3047.	2.0	20
35	Anion templated assembly of [2]catenanes capable of chloride anion recognition in aqueous solvent media. RSC Advances, 2011, 1, 995.	3.6	20
36	Biomolecular Simulations of Halogen Bonds with a GROMOS Force Field. Journal of Chemical Theory and Computation, 2018, 14, 5383-5392.	5.3	20

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37	A New Family of Iron(II)-Cyclopentadienyl Compounds Shows Strong Activity against Colorectal and Triple Negative Breast Cancer Cells. Molecules, 2020, 25, 1592.	3.8	20
38	A DFT and MP2 study of luminescence of gold(I) complexes. Inorganica Chimica Acta, 2006, 359, 3617-3624.	2.4	18
39	Mixed Valence Creutzâ^'Taube Ion Analogues Incorporating Thiacrowns: Synthesis, Structure, Physical Properties, and Computational Studies. Inorganic Chemistry, 2008, 47, 11633-11643.	4.0	17
40	Increased Halide Recognition Strength by Enhanced Intercomponent Preorganisation in Triazolium Containing [2]Rotaxanes. Chemistry - A European Journal, 2013, 19, 17751-17765.	3.3	17
41	Tackling Halogenated Species with PBSA: Effect of Emulating the Ïƒ-Hole. Journal of Chemical Theory and Computation, 2019, 15, 4241-4251.	5.3	15
42	Catalyst control of selectivity in the Câ€“O bond alumination of biomass derived furans. Chemical Science, 2020, 11, 7850-7857.	7.4	15
43	Weak Î·2-Olefin Bonding in Palladium and Platinum Allyl Cationic Complexes Containing Chiral Monodentate Ligands with Î±-Phenyl Methyl Amine Side Chains. Organometallics, 2008, 27, 2949-2958.	2.3	14
44	Trisâ€“thiourea tripodal-based molecules as chloride transmembrane transporters: insights from molecular dynamics simulations. Soft Matter, 2014, 10, 3608.	2.7	14
45	Ionâ€Pair Halogen Bonds in 2â€Haloâ€Functionalized Imidazolium Chloride Receptors: Substituent and Solvent Effects. Chemistry - an Asian Journal, 2017, 12, 586-594.	3.3	14
46	Structure, bonding and reactivity of seven-coordinate allylic Mo(II) and W(II) complexes. Coordination Chemistry Reviews, 2017, 344, 83-100.	18.8	13
47	Photochemistry of Methyltrioxorhenium Revisited:â€‰ A DFT/TD-DFT and CASSCF/MS-CASPT2 Theoretical Study. Organometallics, 2006, 25, 5235-5241.	2.3	12
48	Mapping the Mechanism of Nickelâ€Ferrophite Catalysed Methylation of Baylisâ€“Hillmanâ€Derived S_N2â€² Electrophiles. European Journal of Organic Chemistry, 2009, 2009, 898-903.	2.4	12
49	Interaction of a calix[4]arene derivative with a DOPC bilayer: Biomolecular simulations towards chloride transport. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 890-901.	2.6	12
50	The Hâ‹¯H interaction in the solid state structure of HMn(CO)5. CrystEngComm, 2002, 4, 368-372.	2.6	11
51	Ring Slippage vs Charge Transfer in the Reductive Chemistry of [IndMo(CO)2(Î±-diimine)]+ Cations. Organometallics, 2006, 25, 5223-5234.	2.3	11
52	Modulating the electron-transfer properties of a mixed-valence system through hostâ€“guest chemistry. Chemical Science, 2015, 6, 1334-1340.	7.4	11
53	Synthesis and ligand properties towards gold and silver of the ferrocenylamidobenzimidazole ligand. Journal of Organometallic Chemistry, 2006, 691, 4181-4188.	1.8	10
54	Molecular Dynamics Study of a Heteroditopic-Calix[4]diquinone-Assisted Transfer of KCl and Dopamine Through a Waterâ^'Chloroform Liquidâ^'Liquid Interface. Journal of Physical Chemistry B, 2010, 114, 11173-11180.	2.6	10

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55	pH-Switchability and Second-Order Nonlinear Optical Properties of Monocyclopentadienylruthenium(II)/iron(II) Tetrazoles/Tetrazolates: Synthesis, Characterization, and Time-Dependent Density Functional Theory Calculations. Inorganic Chemistry, 2017, 56, 6849-6863.	4.0	10
56	A new interpretation of the bonding properties and UVâ€“vis spectra of [M3(CO)12] clusters (M=Ru, Os): a TD-DFT study. Comptes Rendus Chimie, 2005, 8, 1477-1486.	0.5	9
57	New Polynuclear Moâ€“Fe Complexes with Ferrocenylamidobenzimidazole Ligands. European Journal of Inorganic Chemistry, 2006, 2006, 4096-4103.	2.0	9
58	Synthesis and differentiation of Î±â€•and Î²â€glycoporphyrin stereoisomers by electrospray tandem mass spectrometry. Rapid Communications in Mass Spectrometry, 2009, 23, 3478-3483.	1.5	9
59	Synthesis of glucopyranos-6â€²-yl purine and pyrimidine isonucleosides as potential cholinesterase inhibitors. Access to pyrimidine-linked pseudodisaccharides through Mitsunobu reaction. Pure and Applied Chemistry, 2016, 88, 363-379.	1.9	9
60	Low-Lying Excited States and Primary Photoproducts of[Os3(CO)10(s-cis-L)] (L=Cyclohexa-1,3-diene,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Density Functional Theory. Chemistry - A European Journal, 2004, 10, 3451-3460.	3.3	8
61	Furanosyl Nucleoside Analogues Embodying Triazole or Theobromine Units as Potential Lead Molecules for Alzheimer's Disease. European Journal of Organic Chemistry, 2018, 2018, 2667-2681.	2.4	8
62	Determination of gas-phase acidities of dimethylphenols: Combined experimental and theoretical study. Journal of the American Society for Mass Spectrometry, 2008, 19, 1590-1599.	2.8	7
63	Cyanideâ€“isocyanide isomers in polynuclear complexes. Reactivity and theoretical studies. Inorganica Chimica Acta, 2003, 356, 297-307.	2.4	6
64	Photoinduced bond cleavage in CH3ReO3: excited state dynamics. New Journal of Chemistry, 2008, 32, 1904.	2.8	6
65	Ruthenium(II) Thiacrown Complexes Incorporating Noninnocent Redox Active Ligands: Synthesis, Electrochemical Properties, and Theoretical Studies. Inorganic Chemistry, 2012, 51, 10483-10494.	4.0	6
66	Binding of RuCp complexes with human apo-transferrin: fluorescence spectroscopy and molecular docking methods. BioMetals, 2021, 34, 1029-1042.	4.1	6
67	Photomodulation of ultrastable hostâ€“guest complexes in water and their application in light-controlled steroid release. Organic Chemistry Frontiers, 0, , .	4.5	6
68	Hydrophosphonylation of aldehydes catalyzed by cyclopentadienyl ruthenium(II) complexes. Molecular Catalysis, 2018, 450, 77-86.	2.0	5
69	Directing self-assembly in solution towards improved cooperativity in Fe(<scp>iii</scp>) complexes with amphiphilic tridentate ligands. Dalton Transactions, 2019, 48, 4239-4247.	3.3	5
70	Synthesis and Exploitation of the Biological Profile of Novel Guanidino Xylofuranose Derivatives**. ChemMedChem, 2022, 17, .	3.2	5
71	Structure, Characterization, and Metal-Complexation Properties of a New Tetraazamacrocycle Containing Two Phenolic Pendant Arms. Helvetica Chimica Acta, 2004, 87, 2613-2628.	1.6	4
72	Optimized Halogen Atomic Radii for PBSA Calculations Using Off-Center Point Charges. Journal of Chemical Information and Modeling, 2021, 61, 3361-3375.	5.4	4

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73	Alumination of aryl methyl ethers: switching between sp² and sp³ Câ€“O bond functionalisation with Pd-catalysis. Chemical Communications, 2021, 57, 11673-11676.	4.1	4
74	Gas-phase interaction between nickel (II) and nitrobenzyl azides: An ESI-MSn study. International Journal of Mass Spectrometry, 2013, 351, 27-36.	1.5	3
75	Accurate Description of Low-Lying Excited States in a Series of Photoreactive Clusters [Os₃(CO)₁₀(Î±-diimine)] by DFT Calculations. Inorganic Chemistry, 2018, 57, 11704-11716.	4.0	3
76	Remote Metal-Arene Ï€ Bonding in Organometallic Complexes: a DFT Study. Collection of Czechoslovak Chemical Communications, 2007, 72, 703-714.	1.0	3
77	Rigid ferrocenophane and its metal complexes with transition and alkaline-earth metal ions. Polyhedron, 2010, 29, 1697-1705.	2.2	2
78	Synthesis of Triazoleâ€Containing Furanosyl Nucleoside Analogues and Their Phosphate, Phosphoramidate or Phoshonate Derivatives as Potential Sugar Diphosphate or Nucleotide Mimetics. ChemPlusChem, 2020, 85, 1676-1691.	2.8	2
79	3. The Halogen bond: Nature and Applications. , 2018, , 81-106.		1
80	Advances in the Computational Modeling of Halogen Bonds in Biochemical Systems. Frontiers in Computational Chemistry, 2018, , 144-183.	0.3	1
81	Transmembrane Anion Transport Mediated by Halogen Bonds: Using Off-Center Charges. Methods in Molecular Biology, 2021, 2315, 273-284.	0.9	0
82	T4 Lysozyme/Halobenzene: A Test System for Modeling Biomolecular Halogen Bonds. , 0, , .		0