Enrique Espinosa

List of Publications by Year
in descending order

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111 papers	5,116 citations	126858 33 h-index	91828 69 g-index
117 all docs	117 docs citations	117 times ranked	4725 citing authors

#	Article	IF	Citations
1	From weak to strong interactions: A comprehensive analysis of the topological and energetic properties of the electron density distribution involving Xâ€“Hâ‹¯Fâ€“Y systems. Journal of Chemical Physics, 2002, 117, 5529-5542.	1.2	1,510
2	The Nature of Halogenâ‹…â‹…â‹…Halogen Interactions: A Model Derived from Experimental Chargeâ€Density Analysis. Angewandte Chemie - International Edition, 2009, 48, 3838-3841.	7.2	343
3	Universal Features of the Electron Density Distribution in Hydrogenâ€Bonding Regions: A Comprehensive Study Involving Hâ‹…â‹…â‹…X (X=H, C, N, O, F, S, Cl, Ï€) Interactions. Chemistry - A European Journal, 2010, 16, 2442-2452.	1.7	228
4	Chalcogen Bonding: Experimental and Theoretical Determinations from Electron Density Analysis. Geometrical Preferences Driven by Electrophilicâ€“Nucleophilic Interactions. Crystal Growth and Design, 2013, 13, 3283-3289.	1.4	154
5	Synthesis of Several Isomeric Tetrathiafulvalene .pi.-Electron Donors with Peripheral Sulfur Atoms. A Study of Their Radical Cations. Journal of Organic Chemistry, 1994, 59, 3307-3313.	1.7	129
6	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	1.7	108
7	Electrostatics at the Origin of the Stability of Phosphateâ€Phosphate Complexes Locked by Hydrogen Bonds. ChemPhysChem, 2012, 13, 1421-1424.	1.0	97
8	The Paradox of Hydrogen-Bonded Anionâ€“Anion Aggregates in Oxoanions: A Fundamental Electrostatic Problem Explained in Terms of ElectrophilicÂ·Â·Â·Nucleophilic Interactions. Journal of Physical Chemistry A, 2015, 119, 183-194.	1.1	94
9	Modulation of the Singletâˆ’Singlet Through-Space Energy Transfer Rates in Cofacial Bisporphyrin and Porphyrinâˆ’Corrole Dyads. Inorganic Chemistry, 2007, 46, 125-135.	1.9	81
10	Synthesis, structure and nuclease properties of several ternary copper(II) peptide complexes with 1,10-phenanthroline. Journal of Inorganic Biochemistry, 2003, 95, 77-86.	1.5	80
11	Charge Density Analysis and Topological Properties of Hal₃-Synthons and Their Comparison with Competing Hydrogen Bonds. Crystal Growth and Design, 2012, 12, 5373-5386.	1.4	78
12	On atomâ€“atom `short contact' bonding interactions in crystals. IUCrJ, 2015, 2, 161-163.	1.0	77
13	Charged versus Neutral Hydrogenâ€Bonded Complexes: Is There a Difference in the Nature of the Hydrogen Bonds?. Chemistry - A European Journal, 2016, 22, 9226-9234.	1.7	77
14	Cocrystal or Salt: Solid State-Controlled Iodine Shift in Crystalline Halogen-Bonded Systems. Crystal Growth and Design, 2015, 15, 3464-3473.	1.4	76
15	Topological Properties of the Electrostatic Potential in Weak and Moderate NÂ·Â·Â·H Hydrogen Bonds. Journal of Physical Chemistry A, 2007, 111, 6425-6433.	1.1	75
16	Coordination behaviour of sulfanilamide derivatives.. Polyhedron, 2000, 19, 991-1004.	1.0	74
17	Dynamic Kinetic Resolution of Racemic Î³-Aryl-Î´-oxoesters. Enantioselective Synthesis of 3-Arylpiperidines. Journal of Organic Chemistry, 2002, 67, 5343-5351.	1.7	70
18	Effect of an external electric field on the dissociation energy and the electron density properties: The case of the hydrogen bonded dimer HFâ‹¯HF. Journal of Chemical Physics, 2009, 130, 044104.	1.2	70

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19	Alkyl- and Aryl-Substituted Corroles. 5. Synthesis, Physicochemical Properties, and X-ray Structural Characterization of Copper Biscorroles and Porphyrinâ˜Corrole Dyads. Inorganic Chemistry, 2004, 43, 7441-7455.	1.9	67
20	Chargeâ€Assisted Halogen Bonding: Donorâ€“Acceptor Complexes with Variable Ionicity. Chemistry - A European Journal, 2013, 19, 14804-14813.	1.7	67
21	Tracing environment effects that influence the stability of anionâ€“anion complexes: The case of phosphateâ€“phosphate interactions. Chemical Physics Letters, 2013, 555, 106-109.	1.2	64
22	Triplet-Triplet Energy Transfer Controlled by the Donor-Acceptor Distance in Rigidly Held Palladium-Containing Cofacial Bisporphyrins. Chemistry - A European Journal, 2005, 11, 3469-3481.	1.7	55
23	Heterobimetallic Complexes of Cobalt(IV) Porphyrinâ˜Corrole Dyads. Synthesis, Physicochemical Properties, and X-ray Structural Characterization. Inorganic Chemistry, 2005, 44, 3972-3983.	1.9	54
24	Room-Temperature Autoconversion of Free-Base Corrole into Free-Base Porphyrin. Angewandte Chemie - International Edition, 2006, 45, 5642-5645.	7.2	46
25	1,1â˜,3,3â˜,6,6â˜,8,8â˜-Octachloro-9,9â˜-bifluorenylidene and Perchloro-9,9â˜-bifluorenylidene, Two Exceedingly Twisted Ethylenes. Journal of Organic Chemistry, 2002, 67, 7175-7178.	1.7	44
26	Fine tuning of the photophysical properties of cofacial diporphyrins via the use of different spacers. Journal of Organometallic Chemistry, 2002, 643-644, 89-97.	0.8	44
27	Periodic Projector Augmented Wave Density Functional Calculations on the Hexachlorobenzene Crystal and Comparison with the Experimental Multipolar Charge Density Model. Journal of Physical Chemistry A, 2011, 115, 14484-14494.	1.1	43
28	Reactivity of copper(II) peptide complexes with bioligands (benzimidazole and creatinine). Polyhedron, 2003, 22, 3255-3264.	1.0	40
29	Interactions of d10 metal ions with hippuric acid and cytosine. X-ray structure of the first cadmium (II)â€“amino acid derivativeâ€“nucleobase ternary compound. Journal of Inorganic Biochemistry, 2001, 85, 173-178.	1.5	37
30	Unprecedented Oxidation of a Phenylglycinol-Derived 2-Pyridone:â€‰ Enantioselective Synthesis of Polyhydroxypiperidines. Organic Letters, 2001, 3, 3257-3260.	2.4	36
31	Toward a reverse hierarchy of halogen bonding between bromine and iodine. Faraday Discussions, 2017, 203, 389-406.	1.6	35
32	Synthesis of Zn N-salicylidene-l-aminoacidatos: X-ray structure of [(N-salicylidene-l-alaninato)(aqua)zinc(II)]Â·0.25H2O and [(N-salicylidene-l-valinato)(aqua)zinc(II)]. Polyhedron, 2000, 19, 673-680.	1.0	34
33	Stabilization of polyiodide chains via anionâ‹¯anion interactions: experiment and theory. CrystEngComm, 2016, 18, 3832-3841.	1.3	34
34	Synthesis, Characterization, and X-ray Crystal Structures of Cyclam Derivatives. 5. Copper(II) Binding Studies of a Pyridine-Strapped 5,12-Dioxocyclam-Based Macrobicycle1. Inorganic Chemistry, 2004, 43, 5572-5587.	1.9	33
35	New Insights into the Complexation of Lead(II) by 1,4,7,10â€Tetrakis(carbamoylmethyl)â€1,4,7,10â€tetraazacyclododecane (DOTAM): Structural, Thermodynamic, and Kinetic Studies. European Journal of Inorganic Chemistry, 2008, 2008, 267-283.	1.0	33
36	Synthesis and characterization of a 1,8-difunctionalized dissymmetrical cyclam copper(II) complex bearing pyridylmethyl and N,N-dimethylcarbamoylmethyl groups. Inorganica Chimica Acta, 2001, 322, 145-149.	1.2	32

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37	The Stereoselective Selfâ€Assembly of Chiral Metalloâ€Organic Cryptophanes. European Journal of Inorganic Chemistry, 2016, 2016, 832-843.	1.0	29
38	Synthesis, Characterization, and X-ray Crystal Structures of Cyclam Derivatives. 8. Thermodynamic and Kinetic Appraisal of Lead(II) Chelation by Octadentate Carbamoyl-Armed Macrocycles1. Inorganic Chemistry, 2005, 44, 7895-7910.	1.9	27
39	Evidence for the Formation of a RuIIIâ€'RuIII Bond in a Ruthenium Corrole Homodimer. Angewandte Chemie - International Edition, 2000, 39, 4051-4053.	7.2	25
40	Zero-Flux Surfaces of the Electrostatic Potential:â€‰ The Border of Influence Zones of Nucleophilic and Electrophilic Sites in Crystalline Environment. Journal of Physical Chemistry A, 2007, 111, 9859-9870.	1.1	25
41	Topological Analysis of the Electron Density Distribution in Perturbed Systems. I. Effect of Charge on the Bond Properties of Hydrogen Fluoride. Journal of Physical Chemistry A, 2005, 109, 6532-6539.	1.1	23
42	Contributions to the application of the transferability principle and the multipolar modeling of HÂatoms: electron-density study ofL-histidinium dihydrogen orthophosphate orthophosphoric acid. I. Acta Crystallographica Section A: Foundations and Advances, 2006, 62, 365-378.	0.3	23
43	New insights into the synthesis of porphyrin-corrole and biscorrole systems. Journal of Porphyrins and Phthalocyanines, 2003, 07, 365-374.	0.4	22
44	A powerful route to C-functionalised tetraazamacrocyclesElectronic supplementary information (ESI) available: synthesis and spectroscopic data of different C-functionalised macrocycles. See http://www.rsc.org/suppdata/cc/b3/b315285e/. Chemical Communications, 2004, , 588.	2.2	22
45	Tuning the Interaction Energy of Hydrogen Bonds: The Effect of the Substituent. Journal of Physical Chemistry A, 2011, 115, 12561-12571.	1.1	22
46	Regioselective N-Functionalization of Tetraazacycloalkanes. Journal of Organic Chemistry, 2005, 70, 7042-7053.	1.7	21
47	Topological Analysis of Hydrogen Bonds and Weak Interactions in Protein Helices via Transferred Experimental Charge Density Parameters. Journal of Physical Chemistry A, 2011, 115, 12895-12904.	1.1	21
48	Activating Chalcogen Bonding (ChB) in Alkylseleno/Alkyltelluroacetylenes toward Chalcogen Bonding Directionality Control. Angewandte Chemie - International Edition, 2020, 59, 23583-23587.	7.2	20
49	StrongÏfâ€Hole Activation on Icosahedral Carborane Derivatives for a Directional Halide Recognition. Angewandte Chemie - International Edition, 2021, 60, 366-370.	7.2	20
50	Synthesis, characterization and X-ray crystal structures of cyclam derivatives. Part IV. 1,4,8,11-Tetraazacyclotetradecane-5,12-dione and its diprotonated forms. New Journal of Chemistry, 2000, 24, 959-966.	1.4	19
51	Synthesis and Physicochemical Characterization of Bis(macrocycles) Involving a Porphyrin and ameso-Substituted Corrole - X-ray Crystal Structure of a [(Free-base) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 182 Td (porphyrin-c 1032-1041.	1.0	18
52	Synthesis, characterization and X-ray crystal structures of cyclam derivatives. Part VI. Proton binding studies of a pyridine-strapped 5,12-dioxocyclam based macrobicycle. New Journal of Chemistry, 2005, 29, 99-108.	1.4	18
53	Sulfur-Incorporating Cyclotriveratrylene Analogues: The Synthesis of Cyclotrithioguaiacylene. Journal of Organic Chemistry, 2011, 76, 1914-1917.	1.7	18
54	9-(2-Methylphenyl)-3,4,5,6,9,10-hexa- hydroxanthene-1,8(2H,7H)-dione. Journal of Chemical Crystallography, 1999, 29, 759-763.	0.5	17

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55	An organic template approach for the synthesis of selectively functionalised tetraazacycloalkanes. Chemical Communications, 2002, , 312-313.	2.2	16
56	Synthesis of new singly metal-metal-bonded heterobinuclear complexes involving a porphyrin and a corrole: X-ray structure of the rhodium tetraphenylporphyrin-tin(2,3,7,13,17,18-hexamethyl-8,12-diethylcorrole) complex. Journal of Porphyrins and Phthalocyanines, 2003, 07, 120-124.	0.4	16
57	X-ray structures and luminescence properties of Co(II) and Co(III) complexes of cofacial diporphyrins. Journal of Porphyrins and Phthalocyanines, 2003, 07, 474-483.	0.4	16
58	Simultaneous Freezing of Chirality and Inâ^'Out Conformation of a Macropentacyclic Cryptand by Protonation. Journal of the American Chemical Society, 2004, 126, 11412-11413.	6.6	16
59	An easy route towards regioselectively difunctionalized cyclens and new cryptands. Chemical Communications, 2006, , 5054.	2.2	16
60	Different ways of interaction between binary copper(II)-Schiff bases (Cuâ€“N-salicylideneserinato) and pyrimidine derivatives. Polyhedron, 2006, 25, 2295-2302.	1.0	16
61	Supramolecular rectangles through directional chalcogen bonding. Chemical Communications, 2021, 57, 4560-4563.	2.2	16
62	Syntheses, characterization and study of the properties of heterobimetallic compounds containing ferrocenyl units X-ray crystal structure of: [Zn(Î·5-C5H5)Fe[(Î·5-C5H4)-CH=N-CH2-CH2-N(CH3)2]Cl2]. Journal of Organometallic Chemistry, 1997, 544, 233-241.	0.8	15
63	Macrotricycles Featuring a Ï€-Basic Tetrahedral Cavity:â€‰ Preference for NH₄⁺ Detected by Electrospray Ionization Mass Spectrometry. Organic Letters, 2007, 9, 2961-2964.	2.4	15
64	The in, out Asymmetric Pseudo-Triple Helical Form of a D₃_h Diaza-Macropentacycle. Journal of Organic Chemistry, 2008, 73, 868-881.	1.7	15
65	Inter-layer charge disproportionation in the dual-layer organic metal (tTTF-I)₂ClO₄with unsymmetrical Iâ‹¯O halogen bond interactions. Dalton Transactions, 2014, 43, 5280-5291.	1.6	15
66	Synthesis and structure of peptideâ€“copper(II)â€“isocytosine ternary complexes. Polyhedron, 2002, 21, 1197-1201.	1.0	14
67	New route to a face-to-face biscorrole free-base and the corresponding heterobimetallic copper(iii)â€“silver(iii) complex. Dalton Transactions, 2004, , 3181-3183.	1.6	13
68	Topological Properties of the Electron Distribution in Hydrogen-bonded Systems. , 0, , 425-451.		13
69	Versatility and dynamics of the copper(i) coordination sphere in sterically hindering tris(pyrazolyl)methane-incorporating macrobicycles. New Journal of Chemistry, 2009, 33, 327.	1.4	13
70	Intermolecular Interaction Energies from Experimental Charge Density Studies. , 2011, , 387-433.		13
71	Chalcogen bonding interactions in chelating, chiral bis(selenocyanates). New Journal of Chemistry, 2021, 45, 76-84.	1.4	13
72	First highly distorted Ï€-extended Fe(II) porphyrin â€“ a unique model to elucidate factors affecting the electrochemical potentials. Journal of Porphyrins and Phthalocyanines, 2004, 08, 1062-1066.	0.4	12

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73	Improved routes for the synthesis of face-to-face bismacrocycles in porphyrin and corrole series. Journal of Porphyrins and Phthalocyanines, 2004, 08, 301-312.	0.4	12
74	Generation of Cryptophanes in Water by Disulfide Bridge Formation. European Journal of Organic Chemistry, 2017, 2017, 3795-3811.	1.2	12
75	From new tricyclic bisaminal derivatives to trans-N,Nâ€²-disubstituted cyclams. Chemical Communications, 2001, , 2728-2729.	2.2	11
76	Understanding Reactivity and Assembly of Dichalcogenides: Structural, Electrostatic Potential, and Topological Analyses of 3H-1,2-Benzodithiol-3-one and Selenium Analogs. Crystal Growth and Design, 2020, 20, 7704-7725.	1.4	11
77	Activating Chalcogen Bonding (ChB) in Alkylseleno/Alkyltelluroacetylenes toward Chalcogen Bonding Directionality Control. Angewandte Chemie, 2020, 132, 23789-23793.	1.6	10
78	Reaction of polyamines with diethyloxalate: a convenient route for the synthesis of tetraazacycloalkanes. Arkivoc, 2006, 2006, 212-233.	0.3	10
79	[(1,4,8,11-Tetraazacyclotetradeca-1,4,8,11-tetrayl)tetraacetamide-Îº6N1,N4,N8,N11,O1,O8]copper(II) sulfate 4.5-hydrate. Acta Crystallographica Section C: Crystal Structure Communications, 2002, 58, m119-m121.	0.4	9
80	The Proton Complex of a Diaza-macropentacycle: Structure, Slow Formation, and Chirality Induction by Ion Pairing with the Optically Active 1,1â€²-Binaphthyl-2,2â€²-diyl Phosphate Anion. Journal of Organic Chemistry, 2008, 73, 7871-7881.	1.7	9
81	Synthesis and Stereochemical Properties of â€œExtendedâ€•Biphenols Bridged by orthoâ€“metaâ€“ and paraâ€Phenylene Spacers. European Journal of Organic Chemistry, 2009, 2009, 6318-6327.	1.2	9
82	Kinetic Control in the Chiral Recognition of Threeâ€Bladed Propellers. Chemistry - A European Journal, 2010, 16, 5706-5711.	1.7	9
83	Polarization of Electron Density Databases of Transferable Multipolar Atoms. Journal of Physical Chemistry A, 2019, 123, 7156-7170.	1.1	9
84	Energetic, Topological and Electric Field Analyses of Cationâ€Cation Nucleic Acid Interactions in Watsonâ€Crick Disposition. ChemPhysChem, 2019, 20, 148-158.	1.0	9
85	Topochemical Polymerization of a Diacetylene in a Chalcogenâ€Bonded (ChB) Assembly. Angewandte Chemie - International Edition, 2022, 61, .	7.2	9
86	Diastereoselective alkylation of 8-phenylmenthyl 2-methylacetoacetate. Preparation of enantiomerically pure 4,4-disubstituted 2-pyrazolin-5-ones. Tetrahedron: Asymmetry, 1997, 8, 1525-1527.	1.8	8
87	Synthesis and crystal structures of palladium(II) complexes of 1,11-bis(2-pyridylmethyl)-1,4,8,11-tetraazacyclotetradecane-5,7-dione. Dalton Transactions RSC, 2001, , 898-901.	2.3	8
88	The Chemoâ€•and Stereoselective Formation of Palladoâ€•and Platinocryptophanes. European Journal of Inorganic Chemistry, 2019, 2019, 2691-2706.	1.0	8
89	Chalcogen Bonding in Co-Crystals: Activation through 1,4-Perfluorophenylene vs. 4,4â€²-Perfluorobiphenylene Cores. Molecules, 2021, 26, 4050.	1.7	8
90	An Opticallyâ€Pure Hemicryptophane as NMR and ECD Responsive Probe for Chloroform. ChemistrySelect, 2016, 1, 2389-2395.	0.7	7

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91	At the Interface of Isomorphous Behavior in a 3 Ã— 3 Isomer Grid of Monochlorobenzamides: Analyses of the Interaction Landscapes via Contact Enrichment Studies. Crystal Growth and Design, 2019, 19, 6141-6158.	1.4	7
92	Comparison of electron density properties in frozen and relaxed electronic distributions. Journal of Computational Chemistry, 2003, 24, 416-421.	1.5	6
93	Synthesis, characterization and X-ray crystal structures of cyclam derivatives. 7. Hydrogen-bond induced allosteric effects and protonation cooperativity in a macrotricyclic bisdioxocyclam receptor. New Journal of Chemistry, 2005, 29, 1121.	1.4	5
94	Strong Ïƒ â€Hole Activation on Icosahedral Carborane Derivatives for a Directional Halide Recognition. Angewandte Chemie, 2021, 133, 370-374.	1.6	4
95	Effect of Substituents on the Molecular Shapes of Ï€â€Basic Macrotricyclic Receptors. European Journal of Organic Chemistry, 2010, 2010, 2701-2708.	1.2	3
96	Dichloro(D-methionine-N,S)platinum(II) at 130â€…K. Acta Crystallographica Section C: Crystal Structure Communications, 2001, 57, 804-806.	0.4	2
97	Topochemical polymerization of a diacetylene in a chalcogenâ€bonded (ChB) assembly. Angewandte Chemie, 0, , .	1.6	2
98	Probing the Electronic Properties and Interaction Landscapes in a Series of N-(Chlorophenyl)pyridinecarboxamides. Crystal Growth and Design, 2022, 22, 3343-3358.	1.4	2
99	N-Iodosaccharinâ€“pyridine co-crystal system under pressure: experimental evidence of reversible twinning. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 436-449.	0.5	2
100	7-Amino-2-methylsulfanyl-1,2,4-triazolo[1,5-a]pyrimidine-6-carboxylic acid as the dimethylformamide and water monosolvates at 293â€…K. Acta Crystallographica Section C: Crystal Structure Communications, 2010, 66, o503-o507.	0.4	1
101	Generation of Stereocenters Around a C3-Symmetric Cyclotriveratrylene Crown. European Journal of Organic Chemistry, 2012, 2012, 2225-2230.	1.2	1
102	A comparative study of two polymorphs of bis(1-hydroxy-2-methylpropan-2-aminium) carbonate. Acta Crystallographica Section C, Structural Chemistry, 2016, 72, 225-229.	0.2	1
103	Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, .	1.7	1
104	2â€²,6â€²-Dimethoxyflavoneâ€“bromoacetic acid (1/1). Acta Crystallographica Section E: Structure Reports Online, 2001, 57, o174-o175.	0.2	0
105	A Powerful Route to C-Functionalized Tetraazamacrocycles.. ChemInform, 2004, 35, no.	0.1	0
106	Improved Routes for the Synthesis of Face-to-face Bismacrocycles in Porphyrin and Corrole Series. ChemInform, 2005, 36, no.	0.1	0
107	Co-crystal versus salt: effect of crystal environment on molecular interactions. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C797-C797.	0.0	0
108	Halogen...halogen interactions from experimental charge-density analysis. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, s240-s240.	0.3	0

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109	N-[3a-(4-Bromophenyl)-8b-hydroxy-6,8-dimethoxy-3-phenyl-2,3,3a,8b-tetrahydro-1H-cyclopenta[b]benzofuran-1-yl]formamide monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o52-o53.	0.2	0
110	Structureâ€“property relationships in halogenated aromatic amides and imides. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C426-C426.	0.0	0
111	Polarizing multipolar atoms: a new toolbox for benchmarking and more. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e77-e77.	0.0	0