Diego M Gil

List of Publications by Year
in descending order

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65	826	516710 16	580821 25
papers	citations	h-index	g-index

65	65	65	920
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ab-initio and DFT calculations on molecular structure, NBO, HOMOâ€“LUMO study and a new vibrational analysis of 4-(Dimethylamino) Benzaldehyde. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 635-643.	3.9	63
2	Recurrent Ï€â€“Ï€ stacking motifs in three new 4,5-dihydropyrazolylâ€“thiazoleâ€“coumarin hybrids: X-ray characterization, Hirshfeld surface analysis and DFT calculations. New Journal of Chemistry, 2020, 44, 14592-14603.	2.8	54
3	Structural, vibrational and electronic characterization of 1-benzyl-3-furoyl-1-phenylthiourea: an experimental and theoretical study. New Journal of Chemistry, 2015, 39, 7459-7471.	2.8	46
4	Quantum chemical studies on molecular structure, spectroscopic (IR, Raman, UVâ€“Vis), NBO and Homoâ€“Lumo analysis of 1-benzyl-3-(2-furoyl) thiourea. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 145, 553-562.	3.9	45
5	Exploring weak intermolecular interactions in thiocyanate-bonded Zn(<scp>ii</scp>) and Cd(<scp>ii</scp>) complexes with methylimidazole: crystal structures, Hirshfeld surface analysis and luminescence properties. RSC Advances, 2018, 8, 23891-23902.	3.6	36
6	Synthesis and structural characterization of perovskite YFeO3 by thermal decomposition of a cyano complex precursor, Y[Fe(CN)6]Â·4H2O. Journal of Thermal Analysis and Calorimetry, 2011, 103, 889-896.	3.6	33
7	New coordination polymers based on 2-methylimidazole and transition metal nitroprusside containing building blocks: synthesis, structure and magnetic properties. New Journal of Chemistry, 2018, 42, 1347-1355.	2.8	26
8	Biofilm inhibition by a new Mn(II) complex with sulfamethoxazole: Synthesis, spectroscopic characterization and crystal structure. Inorganica Chimica Acta, 2015, 436, 16-22.	2.4	25
9	Supramolecular architectures in luminescent Zn(II) and Cd(II) complexes containing imidazole derivatives: Crystal structures, vibrational and thermal properties, Hirshfeld surface analysis and electrostatic potentials. Journal of Molecular Structure, 2017, 1134, 492-503.	3.6	25
10	Intermolecular interactions in antipyrine-like derivatives 2-halo-N-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)benzamides: X-ray structure, Hirshfeld surface analysis and DFT calculations. New Journal of Chemistry, 2020, 44, 19541-19554.	2.8	23
11	Enol-iminoâ€“Keto-enamine Tautomerism in a Diazepine Derivative: How Decisive Are the Intermolecular Interactions in the Equilibrium?. Journal of Organic Chemistry, 2019, 84, 11042-11053.	3.2	22
12	Diethylaminophenyl-based Schiff base Cu(<scp>ii</scp>) and V(<scp>iv</scp>) complexes: experimental and theoretical studies and cytotoxicity assays. New Journal of Chemistry, 2019, 43, 18832-18842.	2.8	22
13	X-ray characterization, Hirshfeld surface analysis, DFT calculations,in vitroandin silicolipoxygenase inhibition (LOX) studies of dichlorophenyl substituted 3-hydroxy-chromenones. New Journal of Chemistry, 2021, 45, 19928-19940.	2.8	22
14	Crystal engineering with pyrazolyl-thiazole derivatives: structure-directing role of Ï€-stacking and Ïƒ-hole interactions. CrystEngComm, 2021, 23, 3276-3287.	2.6	21
15	Lead hexacyanoferrate(II) tetrahydrate: Crystal structure, FTIR spectroscopy and thermal decomposition studies. Polyhedron, 2012, 33, 450-455.	2.2	18
16	Exploration of Brâ‹¯O halogen bonding interactions in dinuclear vanadium(V) complexes with Schiff base ligands. Polyhedron, 2020, 187, 114676.	2.2	18
17	Co(II), Ni(II) and Cu(II) ternary complexes with sulfadiazine and dimethylformamide: Synthesis, spectroscopic characterization, crystallographic study and antibacterial activity. Journal of Molecular Structure, 2019, 1176, 605-613.	3.6	17
18	Crystal structure refinement, spectroscopic study and magnetic properties of yttrium hexacyanoferrate (III). Journal of Molecular Structure, 2011, 1003, 129-133.	3.6	16

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19	Supramolecular self-assembly of a new multi-conformational Schiff base through hydrogen bonds: Crystal structure, spectroscopic and theoretical investigation. Journal of Molecular Structure, 2017, 1133, 24-36.	3.6	15
20	Relevant Ï€-hole tetrel bonding interactions in ethyl 2-triazolyl-2-oxoacetate derivatives: Hirshfeld surface analysis and DFT calculations. CrystEngComm, 2020, 22, 3567-3578.	2.6	15
21	Layered Transition Metal Nitroprussides â€“ Their Preparation, Crystal Structure, and Magnetic Properties. European Journal of Inorganic Chemistry, 2016, 2016, 1690-1696.	2.0	12
22	A New Insight into Non-covalent Interactions in 1,4-Disubstituted 1H-1,2,3-Triazole: Synthesis, X-ray structure, DFT calculations, in vitro Lipoxygenase Inhibition (LOX) and in silico Studies. Journal of Molecular Structure, 2021, 1236, 130283.	3.6	12
23	Crystal structure refinement and vibrational analysis of Y[Co(CN)6]Â·4H2O and its thermal decomposition products. Journal of Molecular Structure, 2013, 1041, 23-28.	3.6	11
24	A detailed exploration of intermolecular interactions in 4-(4-dimethylaminobenzylideneamino)-N-(5-methyl-3-isoxazolyl)benzenesulfonamide and related Schiff bases: Crystal structure, spectral studies, DFT methods, Pixel energies and Hirshfeld surface analysis. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 185, 286-297.	3.9	11
25	A new perfluoromethyl aminoenone derivative and the role of the hydrogen bonding in the intra- and intermolecular interactions. Journal of Fluorine Chemistry, 2018, 208, 36-47.	1.7	11
26	Synthesis, crystal structure, conformational and vibrational properties of 6-acetyl-2,2-dimethyl-chromane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 127, 74-84.	3.9	10
27	Layered vanadyl (IV) nitroprusside: Magnetic interaction through a network of hydrogen bonds. Journal of Solid State Chemistry, 2016, 239, 159-164.	2.9	10
28	Role of Imidazole Coâ€“Ligand in the Supramolecular Network of a Co(II) Complex with Sulfadiazine: Crystal Structure, Hirshfeld Surface Analysis and Energetic Calculations. ChemistrySelect, 2020, 5, 6331-6338.	1.5	9
29	Role of fluorine-fluorine and weak intermolecular interactions in the supramolecular network of a new trifluoromethyl-1,5-benzodiazepine: Crystal structure, Hirshfeld surface analysis and theoretical study. Journal of Fluorine Chemistry, 2021, 242, 109697.	1.7	9
30	Interplay of weak noncovalent interactions in alkoxybenzylidene derivatives of benzohydrazide and acetohydrazide: a combined experimental and theoretical investigation and lipoxygenase inhibition (LOX) studies. CrystEngComm, 2021, 23, 955-971.	2.6	9
31	Layered crystal structure, conformational and vibrational properties of 2,2,2-trichloroethoxysulfonamide: An experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 122-131.	3.9	8
32	DFT calculations of structure and vibrational properties of 2,2,2-trichloroethylacetate, CH3CO2CH2CCl3. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 123, 290-297.	3.9	8
33	Theoretical study on the molecular structure and vibrational properties, NBO and HOMOâ€“LUMO analysis of the POX3 (X=F, Cl, Br, I) series of molecules. Journal of Molecular Structure, 2015, 1081, 536-542.	3.6	8
34	Weak ferromagnetism and superparamagnetic clusters coexistence in YFe1â¯xCoxO3 (0 â‰¤ x â‰¤ 1) perovskites. Materials Research Bulletin, 2017, 94, 472-482.	5.2	8
35	Weak Interactions in Cocrystals of Isoniazid with Glycolic and Mandelic Acids. Crystals, 2021, 11, 328.	2.2	8
36	SYNTHESIS OF Pb2Fe2O5 BY THERMAL DECOMPOSITION OF Pb2[Fe(CN)6].4H2O. Journal of the Chilean Chemical Society, 2010, 55, .	1.2	7

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37	Y[Fe1â˜xCox(CN)6]Â·4H2O (0â©½xâ©½1) solid solutions: Synthesis, crystal structure, thermal decomposition and spectroscopic and magnetic properties. Journal of Molecular Structure, 2012, 1015, 112-117.	3.6	7
38	Synthesis, X-ray characterization and theoretical study of 3a,6:7,9a-diepoxybenzo[de]isoquinoline derivatives: on the importance of Fâ‹¯O interactions. New Journal of Chemistry, 2020, 44, 20167-20180.	2.8	7
39	Revealing new non-covalent interactions in polymorphs and hydrates of Acyclovir: Hirshfeld surface analysis, NCI plots and energetic calculations. Computational and Theoretical Chemistry, 2021, 1197, 113133.	2.5	7
40	Exploring weak intermolecular interactions in two bis-1,3,4-oxadiazoles derivatives: A combined X-ray diffraction, Hirshfeld surface analysis and theoretical studies. Journal of Molecular Structure, 2021, 1232, 130030.	3.6	7
41	Experimental and theoretical vibrational study of the fungicide pyraclostrobin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 259, 119888.	3.9	7
42	Synthesis, molecular structure, spectroscopic and theoretical investigation of 5-chlorosalicylaldehyde-2,4-dinitrophenylhydrazone. Journal of Molecular Structure, 2020, 1205, 127589.	3.6	6
43	Lead nitroprusside: A new precursor for the synthesis of the multiferroic Pb2Fe2O5, an anion-deficient perovskite. Materials Chemistry and Physics, 2013, 141, 355-361.	4.0	5
44	Crystal structure, vibrational and thermal behavior of Ba(NH4)[Co(CN)6]Â·4H2O: A new precursor for the synthesis of hexagonal BaCoO3. Polyhedron, 2014, 73, 51-58.	2.2	5
45	Gas-phase structure of 2,2,2-trichloroethyl chloroformate studied by electron diffraction and quantum-chemical calculations. Physical Chemistry Chemical Physics, 2016, 18, 393-402.	2.8	5
46	A combined experimental and theoretical study of the supramolecular self-assembly of the natural benzopyran 2,2-dimethyl-3-hydroxy-6-acetyl-chromane and its isomeric benzofuran 10,11-dihydro-10-hydroxytremetone. Journal of Molecular Structure, 2017, 1146, 164-178.	3.6	5
47	Raise the anchor! Synthesis, X-ray and NMR characterization of 1,3,5-triazinanes with an axial ‹i›tert‹/i›-butyl group. Organic and Biomolecular Chemistry, 2020, 18, 8386-8394.	2.8	5
48	Vibrational studies (FTIR and Raman), conformational analysis, NBO, HOMOâ€“LUMO and reactivity descriptors of S-methyl thiobutanoate, CH3CH2CH2C(O)SCH3. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 149, 408-418.	3.9	4
49	A detailed study of intermolecular interactions, electronic and vibrational properties of the metal complex bis(uracilato)diammine copper(ii) dihydrate. Journal of Molecular Structure, 2018, 1155, 424-433.	3.6	4
50	Intramolecular sp2-sp3 Disequalization of Chemically Identical Sulfonamide Nitrogen Atoms: Single Crystal X-Ray Diffraction Characterization, Hirshfeld Surface Analysis and DFT Calculations of N-Substituted Hexahydro-1,3,5-Triazines. Crystals, 2020, 10, 369.	2.2	4
51	Deciphering the H-Bonding Preference on Nucleoside Molecular Recognition through Model Copper(II) Compounds. Pharmaceuticals, 2021, 14, 244.	3.8	4
52	An iron(II) complex of trans, trans, trans-bis(azido)bis(4-amino-3,5-bis(2-pyridyl)-1,2,4-triazole): Insight into molecular and supramolecular structures using Hirshfeld surface analysis and DFT studies. Journal of Molecular Structure, 2021, 1235, 130155.	3.6	4
53	Antiparallel Ï€Â·Â·Â·Ï€ and Câ˜HÂ·Â·Â·Hâ˜C contacts in a novel Zn(II) coordination solid involving Ï€-hole tetrel bonding interactions: A combined experimental and theoretical study, Hirshfeld surface analysis, molecular docking and potential drug property. Journal of Molecular Structure, 2022, 1268, 133686.	3.6	4
54	Synthesis, structural and spectroscopic studies of 1-(2-FUROYL)-3-phenylthiourea: a theoretical and experimental approach. Journal of Sulfur Chemistry, 2016, 37, 555-579.	2.0	3

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55	A first exploration of isostructurality in transition metal nitroprussides: X-ray analysis, magnetic properties and DFT calculations. CrystEngComm, 2021, 23, 1158-1171.	2.6	3
56	Role of hydrogen bonds and weak non-covalent interactions in the supramolecular assembly of 9-hydroxyeucaliptol: crystal structure, Hirshfeld surface analysis, and DFT calculations. Journal of Molecular Modeling, 2021, 27, 13.	1.8	3
57	Synthesis, Structure, and Biological Assays of Novel Trifluoromethyldiazepineâ€“Metal Complexes. Australian Journal of Chemistry, 2020, 73, 49.	0.9	3
58	Experimental and theoretical insights into the formation of weak hydrogen bonds and Hâ‹¯H bonding interactions in the solid-state structure of two eucalyptol derivatives. New Journal of Chemistry, 2022, 46, 5690-5704.	2.8	3
59	On the importance of intermolecular interactions of 3-(2,3-dihydroxy-isopentyl)-4-hydroxyacetophenone: Crystal structure, spectroscopic and hirshfeld surface analysis. Journal of Molecular Structure, 2020, 1217, 128393.	3.6	2
60	Synthesis, DFT calculations of structure, vibrational and thermal decomposition studies of the metal complex Pb[Mn(C3H2O4)2(H2O)2]. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 141, 233-238.	3.9	1
61	Structure and bonding of 2,2,2-trichloroethylacetate: An experimental gas phase and computational study. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2016, 71, 1253-1260.	0.7	1
62	Supramolecular, spectroscopic and computational analysis of weak interactions in some thiosemicarbazones derived from 5-acetylbarbituric acid. Journal of Molecular Structure, 2021, 1245, 131031.	3.6	1
63	Novel â€˜main-partâ€™ isostructuralism in metal complexes with 1-methylimidazole: crystal structures, energy calculations and magnetic properties. Dalton Transactions, 2021, 50, 17029-17040.	3.3	1
64	Importance of non-covalent interactions in a nitrile anion metal-complex based on pyridine ligands: A theoretical and experimental approach. Journal of Molecular Structure, 2022, 1261, 132885.	3.6	1
65	Importance of R-CH3â‹¯O tetrel bonding and vinylâ‹¯aryl stacking interactions in stabilizing the crystal packing of 2â€™,4â€™-dihydroxy-3â€™-methoxychalcone: Exploration of antileishmanial activity and molecular docking studies. Journal of Molecular Structure, 2022, 1265, 133357.	3.6	1