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	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
2	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
3	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
4	Antiparallel Ï€Â·Â·Â·Ï€ and Câˆ™HÂ·Â·Â·Hâˆ™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
5	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
6	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
7	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
8	Crystal engineering with pyrazolyl-thiazole derivatives: structure-directing role of Ï€-stacking and Ï*f*-hole interactions. CrystEngComm, 2021, 23, 3276-3287.	2.6	21
9	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
10	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
11	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
12	Weak Interactions in Cocrystals of Isoniazid with Glycolic and Mandelic Acids. Crystals, 2021, 11, 328.	2.2	8
13	Deciphering the H-Bonding Preference on Nucleoside Molecular Recognition through Model Copper(II) Compounds. Pharmaceuticals, 2021, 14, 244.	3.8	4
14	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
15	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
16	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
17	Experimental and theoretical vibrational study of the fungicide pyraclostrobin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 259, 119888.	3.9	7
18	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

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19	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
20	Synthesis, molecular structure, spectroscopic and theoretical investigation of 5-chlorosalicylaldehyde-2,4-dinitrophenylhydrazone. Journal of Molecular Structure, 2020, 1205, 127589.	3.6	6
21	Intermolecular interactions in antipyrine-like derivatives 2-halo-‹i›N‹/i›-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1‹i›H‹/i›-pyrazol-4-yl)benzamides: X-ray structure, Hirshfeld surface analysis and DFT calculations. New Journal of Chemistry, 2020, 44, 19541-19554.	2.8	23
22	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
23	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
24	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
25	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
26	Exploration of Brâ‹¯O halogen bonding interactions in dinuclear vanadium(V) complexes with Schiff base ligands. Polyhedron, 2020, 187, 114676.	2.2	18
27	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
28	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
29	Synthesis, Structure, and Biological Assays of Novel Trifluoromethyldiazepineâ€“Metal Complexes. Australian Journal of Chemistry, 2020, 73, 49.	0.9	3
30	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
31	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
32	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
33	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
34	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
35	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
36	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

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37	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
38	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
39	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
40	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
41	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
42	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
43	Layered vanadyl (IV) nitroprusside: Magnetic interaction through a network of hydrogen bonds. Journal of Solid State Chemistry, 2016, 239, 159-164.	2.9	10
44	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
45	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
46	Layered Transition Metal Nitroprussides â€“ Their Preparation, Crystal Structure, and Magnetic Properties. European Journal of Inorganic Chemistry, 2016, 2016, 1690-1696.	2.0	12
47	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
48	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
49	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
50	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
51	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
52	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
53	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
54	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

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55	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
56	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
57	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
58	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
59	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
60	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
61	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
62	Lead hexacyanoferrate(II) tetrahydrate: Crystal structure, FTIR spectroscopy and thermal decomposition studies. Polyhedron, 2012, 33, 450-455.	2.2	18
63	Crystal structure refinement, spectroscopic study and magnetic properties of yttrium hexacyanoferrate (III). Journal of Molecular Structure, 2011, 1003, 129-133.	3.6	16
64	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
65	SYNTHESIS OF Pb2Fe2O5 BY THERMAL DECOMPOSITION OF Pb2[Fe(CN)6].4H2O. Journal of the Chilean Chemical Society, 2010, 55, .	1.2	7