Gustavo Portalone

List of Publications by Year
in descending order

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111 papers	2,073 citations	249298 26 h-index	325983 40 g-index
112 all docs	112 docs citations	112 times ranked	2163 citing authors

#	Article	IF	Citations
1	Short XÂ·Â·Â·N Halogen Bonds With Hexamethylenetetraamine as the Acceptor. Frontiers in Chemistry, 2021, 9, 623595.	1.8	7
2	A Combined Experimental and Computational Study of Halogen and Hydrogen Bonding in Molecular Salts of 5-Bromocytosine. Molecules, 2021, 26, 3111.	1.7	1
3	Structural, biological and in-silico study of quinoline-based chalcogensemicarbazones. Journal of Molecular Structure, 2020, 1203, 127482.	1.8	6
4	5-Fluorocytosine/Isocytosine Monohydrate. The First Example of Isomorphic and Isostructural Co-Crystal of Pyrimidine Nucleobases. Crystals, 2020, 10, 999.	1.0	7
5	Experimental results and computational insight into sequential reactions of Î²-(2-aminophenyl)-Î±,Î²-ynones with aryl isocyanates/benzoyl isothiocyanate. Organic and Biomolecular Chemistry, 2020, 18, 3177-3189.	1.5	6
6	Crystal structure and Hirshfeld surface analysis of a third polymorph of 2,6-dimethoxybenzoic acid. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1823-1826.	0.2	2
7	Site Selectivity of Halogen Oxygen Bonding in 5- and 6-Haloderivatives of Uracil. Crystals, 2019, 9, 467.	1.0	5
8	6-Methyluracil: a redetermination of polymorph (II). IUCrData, 2019, 4, .	0.1	4
9	Structural and computational study of quinoline-based chalcogensemicarbazones. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e566-e566.	0.0	0
10	Synthesis of potential HIV integrase inhibitors inspired by natural polyphenol structures. Natural Product Research, 2018, 32, 1893-1901.	1.0	3
11	Multifacial Recognition in Binary and Ternary Cocrystals from 5-Halouracil and Aminoazine Derivatives. Crystal Growth and Design, 2018, 18, 5904-5918.	1.4	16
12	Self-assembling of calcium salt of the new DNA base 5-carboxylcytosine. Applied Surface Science, 2017, 407, 297-306.	3.1	3
13	Goldâ€Catalyzed Synthesis of Dibenzo[1,5]diazocines from Î²â€(2â€Aminophenyl)â€Î±,Î²â€ynones. Advanced Synthesis and Catalysis, 2017, 359, 3371-3377.	2.1	27
14	(Chalcogen)semicarbazones and their cobalt complexes differentiate HL-60 myeloid leukaemia cells and are cytotoxic towards tumor cell lines. MedChemComm, 2017, 8, 103-111.	3.5	15
15	Synthesis, structures and electronic properties of Co(III) complexes with 2-quinolinecarboxaldehyde thio- and selenosemicarbazone: A combined experimental and theoretical study. Journal of the Serbian Chemical Society, 2017, 82, 825-839.	0.4	7
16	Role of Weak Hydrogen Bonds and Halogen Bonds in 5-Halo-1,3-dimethyluracils and Their Cocrystalsâ€"A Combined Experimental and Computational Study. Crystal Growth and Design, 2016, 16, 2631-2639.	1.4	15
17	Pro-apoptotic and pro-differentiation induction by 8-quinolinecarboxaldehyde selenosemicarbazone and its Co(<scp>iii</scp>) complex in human cancer cell lines. MedChemComm, 2016, 7, 1604-1616.	3.5	13
18	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil. Journal of Chemical & Engineering Data, 2015, 60, 74-81.	1.0	8

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19	Supramolecular association in proton-transfer adducts containing benzamidinium cations. III. Three molecular salts of 3-methoxy-, 4-methoxy- and 3,4,5-trimethoxybenzoates with benzamidine. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 225-229.	0.2	2
20	Chemisorption of uracil on gold surfaces via density functional theory. Surface Science, 2013, 614, 20-23.	0.8	13
21	The Role of Hydrogen Bonding and Proton Transfer in the Formation of Uracil Networks on the Gold (100) Surface: A Density Functional Theory Approach. Journal of Physical Chemistry C, 2013, 117, 3949-3957.	1.5	31
22	First X-ray diffraction and quantum chemical study of proton-acceptor and proton-donor forms of 5-carboxylcytosine, the last-discovered nucleobase. Journal of Molecular Structure, 2013, 1050, 140-150.	1.8	6
23	Molecular aggregation of novel Zn(II)-salophenpyridyl derivatives. Supramolecular Chemistry, 2013, 25, 709-717.	1.5	7
24	Cytosinium orotate dihydrate. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o14-o15.	0.2	1
25	4-Methoxybenzamidinium bromide. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o56-o56.	0.2	1
26	Benzamidinium 2-methoxybenzoate. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o1114-o1115.	0.2	9
27	4-Methoxybenzamidinium 2,6-dimethoxybenzoate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o268-o269.	0.2	11
28	4-Methoxybenzamidinium hydrogen oxalate monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o3350-o3351.	0.2	1
29	4-Methoxybenzamidinium chloride monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o3083-o3083.	0.2	6
30	4-Methoxybenzamidinium hydrogen sulfate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o3244-o3244.	0.2	3
31	4-Methoxybenzamidinium acetate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o3277-o3277.	0.2	3
32	4-Methoxybenzamidinium nitrate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o3334-o3334.	0.2	1
33	Potassium caffeate/caffeic acid co-crystal: the rat race between the catecholic and carboxylic moieties in an atypical co-crystal. Dalton Transactions, 2012, 41, 14337.	1.6	9
34	Supramolecular association in proton-transfer adducts containing benzamidinium cations. II. Concomitant polymorphs of the molecular salt of 2,6-dimethoxybenzoic acid with benzamidine. Acta Crystallographica Section C: Crystal Structure Communications, 2012, 68, o447-o451.	0.4	9
35	Testing a Variety of Electronic-Structure-Based Methods for the Relative Energies of 5-Formyluracil Crystals. Journal of Chemical Theory and Computation, 2011, 7, 2685-2688.	2.3	23
36	Supramolecular structure of unnatural nucleobases: Revised structure of (2:1) 6-methylisocytosinium dihydrogen monophosphate adduct. Journal of Molecular Structure, 2011, 991, 92-96.	1.8	18

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37	From the X-rays to a reliable â€œlow costâ€•computational structure of caffeic acid: DFT, MP2, HF and integrated molecular dynamicsâ€“X-ray diffraction approach to condensed phases. Journal of Molecular Structure, 2011, 994, 87-96.	1.8	11
38	Solid-phase molecular recognition of cytosine based on proton-transfer reaction. Part II. supramolecular architecture in the cocrystals of cytosine and its 5-Fluoroderivative with 5-Nitrouracil. Chemistry Central Journal, 2011, 5, 51.	2.6	32
39	A new polymorph of 2,6-dimethoxybenzoic acid. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o3394-o3395.	0.2	14
40	Supramolecular association in proton-transfer adducts containing benzamidinium cations. I. Four molecular salts with uracil derivatives. Acta Crystallographica Section C: Crystal Structure Communications, 2010, 66, o295-o301.	0.4	24
41	A Novel 1D-AF Hybrid Organicâ”Inorganic Chromium(II) Methyl Phosphonate Dihydrate: Synthesis, X-Ray Crystal and Molecular Structure, and Magnetic Properties. Inorganic Chemistry, 2010, 49, 7472-7477.	1.9	12
42	Synthesis and Evaluation of New Endomorphin-2 Analogues Containing (Z)-Î±,Î²-Didehydrophenylalanine (Î”Phe) Residues. Journal of Medicinal Chemistry, 2010, 53, 4550-4554.	2.9	30
43	Redox Chemistry of Tetrakis[5,6-di(2-pyridyl)-2,3-pyrazino]porphyrazinatocobalt(II): Isolation and Characterization of Solid Pure CoI, CoII, and CoIIIComplexes. European Journal of Inorganic Chemistry, 2009, 2009, 1600-1607.	1.0	18
44	Solid-Phase Molecular Recognition of Cytosine Based on Proton-Transfer Reaction. Journal of Chemical Crystallography, 2009, 39, 193-200.	0.5	24
45	Redetermination of 2,6-dimethoxybenzoic acid. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o327-o328.	0.2	8
46	A redetermination of 2-nitrobenzoic acid. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o954-o954.	0.2	7
47	Comparison of the Structure and Magnetic Order in a Series of Layered Ni(II) Organophosphonates, Ni[(RPO₃)(H₂O)] (R = C₆H₅, CH₃,) Tj ETQq1 1 0.784314 rgBT /Ove	1.7	8
48	Nicotinohydrazide. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o304-o304.	0.2	4
49	Biguanidinium dichloride. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o683-o683.	0.2	3
50	Redetermination of orotic acid monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o656-o656.	0.2	13
51	Redetermination of 5-iodouracil. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o365-o365.	0.2	5
52	Redetermination of 3-deazauracil. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o1107-o1108.	0.2	3
53	Benzamidinium tetrahydropentaborate sesquihydrate. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o1282-o1283.	0.2	3
54	Acetoguanamine N,N-dimethylformamide solvate. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o1685-o1685.	0.2	5

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55	(3R,5S)-5(3)-Carboxy-3,4,5,6-tetrahydro-2H-1,4-thiazin-4-ium-3(5)-carboxylate. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o636-o636.	0.2	0
56	Evidence of the Facile Hydride and Enolate Addition to the Imine Bond of an Aluminumâ^'Salophen Complex. Inorganic Chemistry, 2007, 46, 9057-9059.	1.9	19
57	The 1:1 cocrystals of the proton-transfer compound dilituric acidâ€"phenylbiguanide monohydrate. Acta Crystallographica Section C: Crystal Structure Communications, 2007, 63, o181-o184.	0.4	11
58	The 1:1 complex of cytosine and 5-fluorouracil monohydrate revisited. Acta Crystallographica Section C: Crystal Structure Communications, 2007, 63, o423-o425.	0.4	12
59	An unusualsynconformation of 5-formyluracil stabilized by supramolecular interactions. Acta Crystallographica Section C: Crystal Structure Communications, 2007, 63, o650-o654.	0.4	14
60	Hydrogen-bonded supramolecular motifs in the 1:1 monohydrated molecular adduct of acetoguanaminium chloride with acetoguanamine and in 2,4,6-triaminopyrimidinediium dichloride dihydrate. Acta Crystallographica Section C: Crystal Structure Communications, 2007, 63, o655-o658.	0.4	17
61	5-[3-(Dimethylamino)propyl]-10,11-dihydro-5H-dibenz[a,d][7]annulen-5-ol. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o746-o747.	0.2	5
62	Redetermination of isocytosine. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o1869-o1871.	0.2	18
63	2,4-Diamino-1,3,5-triazine (guanamine). Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3232-o3232.	0.2	6
64	Asymmetric base pairing in the complex 5-fluorocytosinium chloride/5-fluorocytosine monohydrate. Journal of Chemical Crystallography, 2007, 37, 141-145.	0.5	31
65	Redetermination of 5-fluorocytosine monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o1049-o1051.	0.2	16
66	Redetermination of ammonium oxalate oxalic acid dihydrate. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o4725-o4727.	0.2	4
67	Layered hybrid organicâ€"inorganic Co(II) alkylphosphonates. Synthesis, crystal structure and magnetism of the first two members of the series: Co[(CH3PO3)(H2O)] and Co[(C2H5PO3)(H2O)]. Journal of Solid State Chemistry, 2006, 179, 389-397.	1.4	22
68	Hydrothermal synthesis, structural characterization and magnetic studies of the new pillared microporous ammonium Fe(III) carboxyethylphosphonate: [NH4][Fe2(OH){O3P(CH2)2CO2}2]. Journal of Solid State Chemistry, 2005, 178, 306-313.	1.4	14
69	p-Bromoanilinium chloride. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o3083-o3085.	0.2	7
70	Synthesis and Anti-Rhinovirus Properties of Fluoro-Substituted Flavonoids. Antiviral Chemistry and Chemotherapy, 2005, 16, 267-276.	0.3	40
71	Co(II)n-alkyl phosphonates: examples of hybrid organic-inorganic compounds. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, c358-c358.	0.3	1
72	First example of cocrystals of polymorphic maleic hydrazide. Journal of Chemical Crystallography, 2004, 34, 609-612.	0.5	26

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73	Redetermination of phenylbiguanide hydrochloride. Acta Crystallographica Section E: Structure Reports Online, 2004, 60, o1165-o1166.	0.2	7
74	Cr[(H3Nâ˜'(CH2)2â˜'PO3)(Cl)(H2O)]:Â X-Ray Single-Crystal Structure and Magnetism of a Polar Organicâ˜'Inorganic Hybrid Chromium(II) Organophosphonate. Inorganic Chemistry, 2003, 42, 6345-6351.	1.9	42
75	Ferromagnet. Inorganic Chemistry, 2002, 41, 709-714.	1.9	79
76	Sublimation Thermodynamic Parameters for 5-Fluorouracil and Its 1-Methyl and 1,3-Dimethyl Derivatives from Vapor Pressure Measurements. Journal of Chemical & Engineering Data, 2002, 47, 17-19.	1.0	28
77	1,3-Bridgedp-methyloctahomotetraoxacalix[4]areneâ€"bis-crown-3. Acta Crystallographica Section C: Crystal Structure Communications, 2002, 58, o345-o346.	0.4	0
78	The crystal structure of 3-methyluracil from X-ray powder diffraction data. Journal of Molecular Structure, 2002, 608, 35-39.	1.8	34
79	Synthesis, characterisation and optical properties of symmetrical and unsymmetrical Pt(II) and Pd(II) bis-acetylides. Crystal structure of trans-[Pt(PPh3)2(Cî†Câ€"C6H5)(Cî†Câ€"C6H4NO2)]. Journal of Organometallic Chemistry, 2001, 627, 13-22.	0.8	73
80	Sublimation Enthalpies of Some Methyl Derivatives of Uracil from Vapor Pressure Measurements. Journal of Chemical & Engineering Data, 2000, 45, 242-246.	1.0	40
81	The Effect of Hydrogen Bonding on the Structures of Uracil and Some Methyl Derivatives Studied by Experiment and Theory.. Acta Chemica Scandinavica, 1999, 53, 57-68.	0.7	98
82	Molecular structure of phenylsilane: a study by gas-phase electron diffraction and ab initio molecular orbital calculations. Journal of Organometallic Chemistry, 1998, 560, 183-190.	0.8	19
83	Molecular structure of aniline in the gaseous phase: A concerted study by electron diffraction and ab initio molecular orbital calculations. Structural Chemistry, 1996, 7, 59-71.	1.0	73
84	Synthesis and spectroscopic characterization of new Cu(I) complexes containing triaryl-, tricycloalkylphosphines and heterocyclic anionic or neutral N-donor ligands. Crystal and molecular structure of [(Cy3P)2(pzH)Cu]ClO4Â·CH3OH (Cy=cyclohexyl, pzH=pyrazole). Inorganica Chimica Acta, 1996, 249, 215-229.	1.2	39
85	X-ray Structure and AM1 Studies of the Proton-Transfer Adduct between 2,5-Dihydroxy-p-quinone and 4-(N,N-Dimethylamino)pyridine. The Journal of Physical Chemistry, 1996, 100, 9302-9307.	2.9	6
86	Molecular Structure and Large-Amplitude Motion ofp-Diethynylbenzene from Gas-Phase Electron Diffraction and Theoretical Calculations. The Journal of Physical Chemistry, 1996, 100, 14625-14629.	2.9	8
87	4-Acetamidocyclohexanone Semicarbazone Dihydrate. Acta Crystallographica Section C: Crystal Structure Communications, 1995, 51, 1844-1846.	0.4	0
88	Effect of intermolecular O-H â‹¯ O hydrogen bonding on the molecular structure of phenol: An ab initio molecular orbital study. Structural Chemistry, 1995, 6, 37-45.	1.0	15
89	Synthesis and characterization of derivatives of copper(I) with n-donor ligandsâ€"I. Azole and bis(azolyl)alkane compounds. Crystal structure of nitrato bis(tri-p-tolylphosphine)copper(I). Polyhedron, 1995, 14, 1709-1723.	1.0	30
90	The macromolecular crystallography beamline at ELETTRA. Review of Scientific Instruments, 1995, 66, 1661-1664.	0.6	20

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91	Effect of intermolecular hydrogen bonding on the molecular structures of imidazole and 1,2,4-triazole: A study by ab initio molecular orbital calculations. Structural Chemistry, 1994, 5, 1-7.	1.0	18
92	Molecular structure of ethynylbenzene from electron diffraction and ab initio molecular orbital calculations. Structural Chemistry, 1993, 4, 183-190.	1.0	23
93	(3R,5R)-Tetrahydro-2H-1,4-thiazine-3,5-dicarboxylic acid monohydrate. Acta Crystallographica Section C: Crystal Structure Communications, 1993, 49, 976-978.	0.4	4
94	HF-SCF study of the ground state geometry and harmonic vibrational frequencies of borazine derivatives. Computational and Theoretical Chemistry, 1993, 283, 85-99.	1.5	2
95	Molecular structure of 1,3,5-trifluorobenzene: comparison of the results of two electron diffraction studies. Journal of Molecular Structure, 1992, 269, 367-373.	1.8	12
96	Molecular structure and ring distortion of phenol. An electron diffraction study. Chemical Physics Letters, 1992, 197, 482-488.	1.2	56
97	Ab initio determination of the equilibrium geometry and vibrational frequencies of borazine. Computational and Theoretical Chemistry, 1991, 236, 29-39.	1.5	12
98	Molecular structure of nitrobenzene in the planar and orthogonal conformations. Structural Chemistry, 1990, 1, 107-122.	1.0	133
99	The molecular structure of p-benzenedithiol as determined by electron diffraction. Computational and Theoretical Chemistry, 1989, 186, 185-196.	1.5	17
100	Molecular structure and ring distortions of p-dibromobenzene as determined by electron diffraction. Journal of Molecular Structure, 1988, 176, 71-80.	1.8	11
101	Effect of Intermolecular Hydrogen Bonding on the Molecular and Electronic Stucture of Hydroxybenzenes.. Acta Chemica Scandinavica, 1988, 42a, 460-462.	0.7	14
102	Benzene ring deformation and rotational isomerism in terephthalaldehyde: a study by electron diffraction and molecular orbital calculations. The Journal of Physical Chemistry, 1987, 91, 6120-6127.	2.9	18
103	Molecular structure of p-diaminobenzene in the gaseous phase and in the crystal. The Journal of Physical Chemistry, 1987, 91, 1728-1737.	2.9	55
104	Molecular structure and ring distortions of cyanobenzene: an electron diffraction study. Journal of Molecular Structure, 1987, 160, 97-107.	1.8	31
105	Structural Studies of Benzene Derivatives, XII [1]. The Molecular Structure of 3,5-Dimethylbenzoic Acid in the Crystal, and a Comparison with the Gas Phase Structure of Related Molecules. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1984, 39, 1361-1367.	0.3	2
106	Molecular structure and ring distortions of p-dicyano-benzene in the gas phase and in the crystal. Journal of Molecular Structure, 1984, 112, 141-157.	1.8	57
107	Molecular structure and ring distortions of fluorobenzene: an electron diffraction study, and a comparison with other experimental and ab initio MO results. Journal of Molecular Structure, 1984, 118, 53-61.	1.8	60
108	Molecular structure and ring distortions of p-diiso-cyanobenzene in the gaseous phase and in the crystal. Journal of Molecular Structure, 1984, 125, 19-32.	1.8	29

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109	Molecular Structures of p-Methylsulphonylbenzoic Acid and Methylphenylsulphone: Comparison of X-Ray and Electron Diffraction Results. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1984, 39, 607-609.	0.3	7
110	Research on african medicinal plantsâ€"IV. Tetrahedron, 1983, 39, 323-329.	1.0	45
111	Effects of Through-Conjugation on the Molecular Structure of p-Nitroaniline [1]. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1982, 37, 1309-1311.	0.3	45