Mauricio Federico Erben

List of Publications by Citations

128 papers	1,943 citations	23 h-index	36 g-index
131 ext. papers	2,148 ext. citations	3.1 avg, IF	4.9 L-index

#	Paper	IF	Citations
128	A review on the chemistry, coordination, structure and biological properties of 1-(acyl/aroyl)-3-(substituted) thioureas. *Journal of Sulfur Chemistry*, **2014**, 35, 318-355	2.3	145
127	Intermolecular interactions in crystalline 1-(adamantane-1-carbonyl)-3-substituted thioureas with Hirshfeld surface analysis. *CrystEngComm*, **2015**, 17, 7551-7563	3.3	59
126	Recent developments in chemistry, coordination, structure and biological aspects of 1-(acyl/aroyl)-3-(substituted) thioureas. *Research on Chemical Intermediates*, **2017**, 43, 3053-3093	2.8	52
125	Anomeric and mesomeric effects in methoxycarbonylsulfenyl chloride, CH(3)OC(O)SCl: an experimental and theoretical study. *Inorganic Chemistry*, **2002**, 41, 1064-71	5.1	51
124	Intra- and intermolecular hydrogen bonding and conformation in 1-acyl thioureas: an experimental and theoretical approach on 1-(2-chlorobenzoyl)thiourea. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 143, 59-66	4.4	45
123	Synthesis, structural and vibrational properties of 1-(adamantane-1-carbonyl)-3-halophenyl thioureas. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 102, 408-13	4.4	43
122	Supramolecular self-assembly of a coumarine-based acylthiourea synthon directed by π-stacking interactions: Crystal structure and Hirshfeld surface analysis. *Journal of Molecular Structure*, **2016**, 1111, 76-83	3.4	42
121	Toward an intimate understanding of the structural properties and conformational preference of oxoesters and thioesters: gas and crystal structure and conformational analysis of dimethyl monothiocarbonate, CH3OC(O)SCH3. *Journal of Organic Chemistry*, **2006**, 71, 616-22	4.2	40
120	NH?SC hydrogen bond in O-alkyl N-methoxycarbonyl thiocarbamates, ROC(S)N(H)C(O)OCH3 (R=CH3, CH3CH2). *Polyhedron*, **2009**, 28, 937-946	2.7	38
119	Fluoroformyl trifluoroacetyl disulfide, FC(O)SSC(O)CF3: synthesis, structure in solid and gaseous states, and conformational properties. *Inorganic Chemistry*, **2005**, 44, 7070-7	5.1	38
118	Dramatic changes in geometry after ionization: experimental and theoretical studies on the electronic properties of fluorocarbonyl (mono-, di-, and tri-) sulfur compounds. *Inorganic Chemistry*, **2002**, 41, 3740-8	5.1	38
117	Competing intramolecular NHOC hydrogen bonds and extended intermolecular network in 1-(4-chlorobenzoyl)-3-(2-methyl-4-oxopentan-2-yl) thiourea analyzed by experimental and theoretical methods. *Chemical Physics*, **2014**, 431-432, 39-46	2.3	37
116	Synthesis, spectroscopic study, X-ray crystallography and ab initio calculations of the two new phosphoramidates: C6H5OP(O)(NHC6H11)2 and [N(CH3)(C6H11)]P(O)(2-C5H4N-NH)2. *Journal of Molecular Structure*, **2008**, 874, 178-186	3.4	36
115	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	3.6	35
114	[Chloro(difluoro)acetyl]phosphoramidic acid dichloride ClF2CC(O)NHP(O)Cl2, synthesis, vibrational and NMR spectra and theoretical calculations. *Journal of Molecular Structure*, **2008**, 886, 66-71	3.4	35
113	Synthesis, X-ray crystal structure, thermal behavior and spectroscopic analysis of 1-(1-naphthoyl)-3-(halo-phenyl)-thioureas complemented with quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 150, 409-18	4.4	34
112	Preparation and properties of methoxycarbonylsulfenyl isocyanate, CH(3)OC(O)SNCO. *Journal of Organic Chemistry*, **2007**, 72, 9074-80	4.2	33

111	Current developments in chemistry, coordination, structure and biological aspects of 1-(acyl/aroyl)-3- (substituted)thioureas: advances Continue *Journal of Sulfur Chemistry*, **2019**, 40, 312-350	2.3	32
110	Structural and vibrational study on N-(biphenyl-2-thiocarbamoyl)-4-phenylcarboxamide. *Journal of Molecular Structure*, **2011**, 985, 57-62	3.4	30
109	Trifluoromethyl chlorosulfonate, CF3OSO2Cl: gas phase and crystal structure, conformation and vibrational analysis studied by experimental and theoretical methods. *Inorganic Chemistry*, **2003**, 42, 7297-303	5.1	28
108	Effect of fluorine substitution on the crystal structures and vibrational properties of phenylthiourea isomers. *Journal of Molecular Structure*, **2010**, 982, 91-99	3.4	27
107	Understanding the conformational changes and molecular structure of furoyl thioureas upon substitution. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2017**, 176, 8-17	4.4	25
106	Synthesis, structural and vibrational properties of 1-(4-Fluorobenzoyl)-3-(isomeric fluorophenyl)thioureas. *Journal of Molecular Structure*, **2011**, 1000, 49-57	3.4	24
105	Vibrational spectra and molecular structure of isomeric 1-(adamantan-1-ylcarbonyl)-3-(dichlorophenyl)thioureas. *Journal of Molecular Structure*, **2017**, 1129, 283-291	3.4	23
104	Synthesis, crystal X-ray diffraction structure, vibrational properties and quantum chemical calculations on 1-(4-(4-Fluorobenzamido)phenyl)-3-(4-fluorobenzoyl)thiourea. *Journal of Molecular Structure*, **2010**, 984, 240-245	3.4	23
103	Syntheses, spectroscopic study and X-ray crystallography of some new phosphoramidates and lanthanide(III) complexes of N-(4-nitrobenzoyl)-N',N''-bis(morpholino)phosphoric triamide. *Acta Crystallographica Section B: Structural Science*, **2010**, 66, 441-50		23
102	On the roles of close shell interactions in the structure of acyl-substituted hydrazones: An experimental and theoretical approach. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2016**, 157, 138-145	4.4	22
101	Methyl Fluorocarbonyl Disulfide (FC(O)SSMe): A Theoretical Study on the Structural and Conformational Properties of Its Neutral Ground State and Lowest-Lying Cationic State. *Helvetica Chimica Acta*, **2003**, 86, 2379-2395	2	22
100	Novel Guanidine Compound against Multidrug-Resistant Cystic Fibrosis-Associated Bacterial Species. *Molecules*, **2018**, 23,	4.8	21
99	Hydrogen bonding interactions between glucose, and methacrylic acid. *Structural Chemistry*, **2011**, 22, 1347-1352	1.8	21
98	Novel C-2 Symmetric Molecules as Glucosidase and Amylase Inhibitors: Design, Synthesis, Kinetic Evaluation, Molecular Docking and Pharmacokinetics. *Molecules*, **2019**, 24,	4.8	20
97	He I photoelectron spectra and valence synchrotron photoionization for XC(O)SCl (X = F, Cl) compounds. *Journal of Physical Chemistry A*, **2008**, 112, 2228-34	2.8	20
96	Study of the Ionic Fragmentation of Shallow- and Core-Excited Fluorocarbonylsulfenyl Chloride, FC(O)SCl: Observation of a New Three-Body Dissociation Mechanism. *Journal of Physical Chemistry A*, **2004**, 108, 3938-3946	2.8	20
95	Trifluoromethyl Chloroformate, ClC(O)OCF3: Structure, Conformation, and Vibrational Analysis Studied by Experimental and Theoretical Methods *Journal of Physical Chemistry A*, **2004**, 108, 699-706	2.8	20
94	Close insight into the nature of intermolecular interactions in dihydropyrimidine-2(1H)-thione derivatives. *CrystEngComm*, **2017**, 19, 1495-1508	3.3	19

93	Exploration of carboxy pyrazole derivatives: Synthesis, alkaline phosphatase, nucleotide pyrophosphatase/phosphodiesterase and nucleoside triphosphate diphosphohydrolase inhibition studies with potential anticancer profile. *European Journal of Medicinal Chemistry*, **2018**, 156, 461-478	6.8	19
92	The role of substituents in the molecular and crystal structure of 1-(adamantane-1-carbonyl)-3-(mono)- and 3,3-(di) substituted thioureas. *Journal of Molecular Structure*, **2014**, 1065-1066, 150-159	3.4	19
91	Synthesis, crystal structure and spectroscopic properties of a novel carbacylamidophosphate: N-(3-nitrobenzoyl)-N',N''-bis(tert-butyl)phosphoric triamide. *Acta Crystallographica Section B: Structural Science*, **2009**, 65, 502-8		19
90	Evidence of site-specific fragmentation on thioacetic acid, CH3C(O)SH, irradiated with synchrotron radiation around the S 2p and O 1s regions. *Journal of Physical Chemistry A*, **2006**, 110, 875-83	2.8	19
89	Twisted imide bond in noncyclic imides. Synthesis and structural and vibrational properties of N,N-bis(furan-2-carbonyl)-4-chloroaniline. *Journal of Organic Chemistry*, **2012**, 77, 4688-95	4.2	18
88	Conformation of N,N?-bis (2,6-dimethylmorpholino), N?-dichloroacetyl phosphoric triamide: CHCl2C(O)NHP(O)[2,6(CH3)2(NC4H6O)]2. NMR and ab initio studies. *Journal of Molecular Structure*, **2007**, 840, 66-70	3.4	18
87	Synthesis, conformational and NQR analysis of phosphoric triamides containing the P(O)[N]3 skeleton. *Journal of Molecular Structure*, **2012**, 1023, 18-24	3.4	17
86	HeI photoelectron and valence synchrotron photoionization studies of the thioester molecule CH3C(O)SCH3: evidence of vibronic structure. *Journal of Physical Chemistry A*, **2008**, 112, 5947-53	2.8	17
85	Vibrational studies of N-trifluoroacetyl-phosphoramidic acid dichloride [CF3C(O)NHP(O)Cl2] and N-trichloroacetyl-phosphoramidic acid dichloride [CCl3C(O)NHP(O)Cl2]. *Vibrational Spectroscopy*, **2008**, 46, 107-114	2.1	17
84	Ionic fragmentation on ClC(O)SCl. Evidence of a highly charged molecular ion and confirmation of unusual dissociation mechanisms for halocarbonylsulfenyl chlorides. *Journal of Physical Chemistry A* , **2005**, 109, 304-13	2.8	17
83	Synthesis of aryl pyrazole via Suzuki coupling reaction, in vitro mushroom tyrosinase enzyme inhibition assay and in silico comparative molecular docking analysis with Kojic acid. *Bioorganic Chemistry*, **2018**, 79, 293-300	5.1	17
82	Structural effects and hydrogen bonds on N,N?-di(methoxycarbonylsulfenyl)urea, [CH3OC(O)SNH]2CO, studied by experimental and theoretical methods. *Journal of Molecular Structure*, **2009**, 918, 146-153	3.4	16
81	Dissociative photoionization of methyl thiocyanate, CH3SCN, in the proximity of the sulfur 2p edge. *Journal of Physical Chemistry A*, **2009**, 113, 564-72	2.8	16
80	Dissociative photoionization of methoxycarbonylsulfenyl chloride, CH3OC(O)SCl, following sulfur 2p, chlorine 2p, and oxygen 1s excitations. *Journal of Physical Chemistry A*, **2007**, 111, 8062-71	2.8	16
79	Matrix photochemistry, photoelectron spectroscopy, solid-phase structure, and ring strain energy of beta-propiothiolactone. *Journal of Physical Chemistry A*, **2009**, 113, 3662-72	2.8	15
78	Perchloromethyl mercaptan, CCl3SCl, excited with synchrotron radiation in the proximity of the sulfur and chlorine 2p edges: dissociative photoionization of highly halogenated species. *Journal of Physical Chemistry A*, **2009**, 113, 9624-32	2.8	15
77	Synthesis and characterization of the first phosphonic diamide containing thiazolyl groups: Structural properties and tautomeric equilibrium. *Journal of Molecular Structure*, **2010**, 978, 67-73	3.4	15
76	Structural study of a novel acetylide-thiourea derivative and its evaluation as a detector of benzene. *Journal of Molecular Structure*, **2017**, 1139, 353-361	3.4	14

75	Vibrational spectra, crystal structures, constitutional and rotational isomerism of FC(O)SCN and FC(O)NCS. *Inorganic Chemistry*, **2010**, 49, 11142-57	5.1	14
74	Conformational and structural determination of F(2)NC(O)F and F(2)NC(O)NCO. A joint experimental and theoretical study. *Journal of Physical Chemistry A*, **2009**, 113, 13029-35	2.8	14
73	An investigation of supramolecular synthons in 1,2,4-triazole-3(4H)-thione compounds. X-ray crystal structures, energetic and Hirshfeld surface analysis. *Journal of Molecular Structure*, **2019**, 1195, 796-806	3.4	13
72	Synthesis, conformational studies and NBO analysis of (4-chloro-3,5-dimethyl-1H-pyrazol-1-yl)(p-tolyl)methanone. *Journal of Molecular Structure*, **2019**, 1191, 152-157	3.4	13
71	DFT calculations on the hydrogen bonding interactions between adrenaline and trimethoxysilylpropylamine. *Main Group Chemistry*, **2012**, 11, 275-284	0.6	13
70	Matrix photochemistry at low temperatures and spectroscopic properties of gamma-butyrothiolactone. *Journal of Physical Chemistry A*, **2010**, 114, 9462-70	2.8	12
69	Synthesis, Structure and Conformational Properties of Fluoroformylchlorodifluoroacetyl Disulfide, FC(O)SSC(O)CF2Cl: Conformational Transferability in □C(O)SSC(O)□Compounds. *European Journal of Inorganic Chemistry*, **2006**, 2006, 4418-4425	2.3	12
68	Elucidation of the Average Molecular Structure of Argentinian Asphaltenes. *Energy & Fuels*, **2019**, 33, 2950-2960	4.1	11
67	The Structure and Conformation of (CH3)3 CSNO. *Chemistry - A European Journal*, **2015**, 21, 10436-42	4.8	11
66	Conformational behavior of CH3OC(O)SX (X = CN and SCN) pseudohalide congeners. A combined experimental and theoretical study. *Journal of Physical Chemistry A*, **2010**, 114, 3703-12	2.8	11
65	Dissociation dynamics of highly charged molecular ions of FC(O)SCl. *Journal of Electron Spectroscopy and Related Phenomena*, **2007**, 155, 64-69	1.7	10
64	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	3.6	10
63	Gas and crystal structures of CCl2FSCN. *Journal of Molecular Structure*, **2017**, 1132, 175-180	3.4	9
62	Photofragmentation Mechanisms of Chlorosulfonyl Isocyanate, ClSO2NCO, Excited with Synchrotron Radiation between 12 and 550 eV. *Journal of Physical Chemistry A*, **2015**, 119, 8021-30	2.8	9
61	Structures of Trichloromethyl Thiocyanate, CCl3 SCN, in Gaseous and Crystalline State. *ChemPhysChem*, **2016**, 17, 1463-7	3.2	9
60	Speciation of sulphur in asphaltenes and resins from Argentinian petroleum by using XANES spectroscopy. *Fuel*, **2019**, 256, 115952	7.1	9
59	Evidence for the formation of an interstellar species, HCS+, during the ionic fragmentation of methyl thiofluoroformate, FC(O)SCH3, in the 100-1000 eV region. *Journal of Physical Chemistry A*, **2010**, 114, 12353-61	2.8	9
58	Outermost and inner-shell electronic properties of ClC(O)SCH2CH3 studied using HeI photoelectron spectroscopy and synchrotron radiation. *Journal of Physical Chemistry A*, **2011**, 115, 5307-18	2.8	9

57	Synthesis, spectroscopy, computational study and prospective biological activity of two novel 1,3,2-diazaphospholidine-2,4,5-triones. *Polyhedron*, **2009**, 28, 541-547	2.7	9
56	A Mixed Ligand Platinum(II) Complex: Spectral Analysis, Crystal Structure, Steric Demand of the Ligand, and Bioactivity of cis-[Pt(PPh3)2(L1-O,S)]PF6 (L1-O,S = N,N-Morpholine-N?-benzoylthiourea). *European Journal of Inorganic Chemistry*, **2019**, 2019, 2583-2590	2.3	8
55	Ionic fragmentation mechanisms of 2,2,2-trifluoroethanol following excitation with synchrotron radiation. *ChemPhysChem*, **2015**, 16, 322-30	3.2	8
54	One-pot synthesis, quantum chemical calculations and X-ray diffraction studies of thiazolyl-coumarin hybrid compounds. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2018**, 198, 290-296	4.4	8
53	Interstellar H3+ and HCS+ ions produced in the dissociative photoionization process of CH3C(O)SCH3 in the proximity of the sulfur 2p, carbon 1s, and oxygen 1s edges. *Journal of Physical Chemistry A*, **2012**, 116, 2571-82	2.8	8
52	Study of the photodissociation process of ClC(O)SCH3 using both synchrotron radiation and HeI photoelectron spectroscopy in the valence region. *Journal of Physical Chemistry A*, **2010**, 114, 8049-55	2.8	8
51	Anomeric Interactions in Pentafluoroethylimidosulfurous Dichloride, CF3CF2N=SCl2: Structural, Conformational and Configurational Properties in the Gaseous and Condensed Phases. *European Journal of Inorganic Chemistry*, **2007**, 2007, 3535-3542	2.3	8
50	Chlorodifluorothioacetic Acid, CF2ClC(O)SH: Synthesis, Characterization, X-ray Structure and Conformational Properties. *European Journal of Organic Chemistry*, **2007**, 2007, 4917-4926	3.2	8
49	The structure of chloromethyl thiocyanate, CH2ClSCN, in gas and crystalline phases. *Physical Chemistry Chemical Physics*, **2015**, 17, 15805-12	3.6	7
48	Conformational properties of ethyl- and 2,2,2-trifluoroethyl thionitrites, (CX□CH5NO, X = H and F). *Journal of Physical Chemistry A*, **2015**, 119, 1524-33	2.8	7
47	A combined experimental and theoretical study of the tautomeric and conformational properties of (5-phenyl-tetrazol-2-yl)-acetic acid methyl ester. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 150, 1-8	4.4	7
46	Electronic properties and dissociative photoionization of thiocyanates. Part II. Valence and shallow-core (sulfur and chlorine 2p) regions of chloromethyl thiocyanate, CH2ClSCN. *Journal of Physical Chemistry A*, **2012**, 116, 231-41	2.8	7
45	Convenient synthesis of carbamates, S-alkyl thiocarbamates, and N,N?-disubstituted urea derivatives of methoxycarbonylsulfenyl isocyanate. *Tetrahedron Letters*, **2011**, 52, 5352-5354	2	7
44	Perfluoromethyl fluorocarbonyl peroxide, CF3OOC(O)F: structure, conformations, and vibrational spectra studied by experimental and theoretical methods. *Inorganic Chemistry*, **2003**, 42, 3079-85	5.1	7
43	Ibuprofen-thiadiazole hybrid compounds: Synthesis, vibrational analysis and molecular structure of 5-(1-(4-isobutylphenyl)ethyl)-1,3,4-thiadiazol-2-amine hydrochloride. *Journal of Molecular Structure*, **2019**, 1179, 11-17	3.4	7
42	An intramolecular 1,5-chalcogen bond on the conformational preference of carbonyl thiocarbamate species. *New Journal of Chemistry*, **2020**, 44, 5243-5253	3.6	6
41	Electronic properties of fluorosulfonyl isocyanate, FSO2NCO: a photoelectron spectroscopy and synchrotron photoionization study. *Journal of Physical Chemistry A*, **2013**, 117, 9179-88	2.8	6
40	Conformational transferability of the sulfenyl carbonyl group -SC(O)- in cyclic thioesters. *Journal of Physical Chemistry A*, **2013**, 117, 5706-14	2.8	6

39	Spectroscopic characterization and constitutional and rotational isomerism of ClC(O)SCN and ClC(O)NCS. *Journal of Physical Chemistry A*, **2013**, 117, 2383-99	2.8	6
38	Methoxycarbonyl trifluoromethyl disulfide, CH3OC(O)SSCF3: synthesis, structure and conformational properties. *New Journal of Chemistry*, **2010**, 34, 1365	3.6	6
37	Conformational and crystal structure of acyl thiourea compounds: The case of the simple (2,2-dimethyl-propionyl) thiourea derivative. *Journal of Molecular Structure*, **2020**, 1215, 128227	3.4	6
36	Dissociative photoionization of methyl thiochloroformate, ClC(O)SCH3, following sulfur 2p, chlorine 2p, carbon 1s, and oxygen 1s excitations. *Journal of Physical Chemistry A*, **2012**, 116, 7498-507	2.8	5
35	Determination of heats of tautomerization nitrile-ketenimine by mass spectrometry. *European Journal of Mass Spectrometry*, **2011**, 17, 125-43	1.1	5
34	Molecular and electronic structure of Ɛvalerothiolactone. *Journal of Physical Chemistry A*, **2010**, 114, 12540-7	2.8	5
33	Comment on "Structural and vibrational studies on 1-(5-Methyl- [1,3,4] thiadiazol-2-yl)-pyrolidin-2-ol" [Spectrochimica Acta Part A, 152 (2016) 252-261]. The importance of intramolecular OH?N hydrogen bonding in the conformational properties of thiadiazol-pyrrolidin-2-ol bearing species. *Spectrochimica Acta - Part A: Molecular and Biomolecular*	4.4	5
32	Matrix isolation study of the conformations and photochemistry of S-ethyl fluorothioformate, FC(O)SCH2CH3. *Journal of Physical Chemistry A*, **2014**, 118, 11193-203	2.8	4
31	Conformational preference of chlorothioformate species: molecular structure of ethyl chlorothioformate, ClC(O)SCH2CH3, in the solid phase and NBO analysis. *Acta Crystallographica Section B: Structural Science*, **2011**, 67, 350-6		4
30	Crystal structure, spectroscopic characterization and Hirshfeld surface analysis of aqua-dichlorido-{-[(pyridin-2-yl)methyl-idene]aniline}copper(II) monohydrate. *Acta Crystallographica Section E: Crystallographic Communications*, **2020**, 76, 148-154	0.7	4
29	The effect of chalcogen substitution on the structure and spectroscopy of 4,7-dimethyl-2H-chromen-2-one/thione analogues. *New Journal of Chemistry*, **2017**, 41, 5770-5783	3.6	3
28	Vibrational properties, crystal X-ray diffraction structure and quantum chemical calculations on a divalent sulfur substituted phthalimide: 1H-Isoindole-1,3(2H)-dione, 2-[(methoxycarbonyl)thio]. *Journal of Molecular Structure*, **2010**, 975, 227-233	3.4	3
27	On the conformational behavior of O,O-dimethyl phosphamidothioate (SP(OCH3)2NH2). *Journal of Molecular Structure*, **2005**, 734, 107-113	3.4	3
26	Theoretical investigation on the conformational space of perfluorohydroxylamine, F2NOF. *Chemical Physics*, **2005**, 308, 193-198	2.3	3
25	Recent trends in chemistry, structure, and various applications of 1-acyl-3-substituted thioureas: a detailed review.. *RSC Advances*, **2022**, 12, 12710-12745	3.7	3
24	Formation of HCO and HCS Ions in the Photodissociation of CHOC(S)SCH under VUV Synchrotron Radiation. *Journal of Physical Chemistry A*, **2019**, 123, 6674-6682	2.8	2
23	Electronic properties of FC(O)SCH2CH3. a combined helium(I) photoelectron spectroscopy and synchrotron radiation study. *Journal of Physical Chemistry A*, **2014**, 118, 5950-60	2.8	2
22	Electronic Properties and Dissociative Photoionization of Thiocyanates, Part III. The Effect of the Group's Electronegativity in the Valence and Shallow-Core (Sulfur and Chlorine 2p) Regions of CClSCN and CClFSCN. *Journal of Physical Chemistry A*, **2017**, 121, 9201-9210	2.8	2

21	Photoexcitation, photoionization, and photofragmentantion of CF3CF2CF2C(O)Cl using synchrotron radiation between 13 and 720 eV. *Journal of Physical Chemistry A*, **2015**, 119, 1894-905	2.8	2
20	N,N-Difluoro-O-trifluoromethyl-hydroxylamine, CF3ONF2: conformation and vibrational analysis studied by experimental and theoretical methods. *Journal of Molecular Structure*, **2004**, 692, 63-70	3.4	2
19	On the planarity of the cyclobutane ring in the crystal of dimethyl 2,4-bis(3,4-dimethoxyphenyl)cyclobutane-1,3-dicarboxylate: a natural bond orbital and Hirshfeld surface analysis study. *New Journal of Chemistry*, **2020**, 44, 15515-15525	3.6	2
18	Valence and Inner Electronic Excitation, Ionization, and Fragmentation of Perfluoropropionic Acid. *Journal of Physical Chemistry A*, **2018**, 122, 9842-9850	2.8	2
17	Investigation of stable solid diazonium salt by molecular structure, Hirshfeld surface analysis, optical and electrochemical studies, and applications. *Journal of Molecular Modeling*, **2021**, 27, 296	2	2
16	Intra- and intermolecular NHO=C hydrogen bonds in 1-acyl urea compounds: Synthesis, X-ray structure, conformational and Hirshfeld surface analyses of 1-(2,3-dichlorophenyl)-3-pivaloylurea. *Journal of Molecular Structure*, **2021**, 1245, 131271	3.4	2
15	Stannathianes as activated polythiols for the synthesis of functionalized macrocyclic polythiolactones. *Tetrahedron Letters*, **2017**, 58, 1484-1486	2	1
14	Interplay between Conformation and Crystal Packing in Aryl Propargyl Ethers: Structural and Spectroscopic Properties of 2-(prop-2-yn-1-yloxy)acene Derivatives. *ChemistrySelect*, **2019**, 4, 9927-9933	1.8	1
13	The ionic nature of methylsulfur trichloride species. *Inorganic Chemistry Communication*, **2012**, 26, 66-68	3.1	1
12	Structure, conformational properties and matrix photochemistry of S-(tert-butyl)trifluorothioacetate CF3C(O)SC(CH3)3. *New Journal of Chemistry*, **2020**, 44, 14568-14577	3.6	1
11	Synthesis and Structure of 4-Chloro-2-{[5-(diethylamino)-2-hydroxybenzylidene]amino}phenol and Its Metal Complexes. *Russian Journal of General Chemistry*, **2020**, 90, 2376-2380	0.7	0
10	Synthesis, conformation and Hirshfeld surface analysis of benzoxazole methyl ester as a versatile building block for heterocycles. *Heliyon*, **2021**, 7, e08042	3.6	0
9	A Dual Approach on Experimental, Theoretical Insight of Structural Elucidation, Hirshfeld Surface Analysis, Optical and Electrochemical Properties of Acyl Thiourea-Ethynyl Hybrid Derivatives.. *Journal of Chemical Crystallography*, **2022**, 1-14	0.5	0
8	Electronic Properties and Ionic Photodissociation of Thionitrite Compounds RSNO [R=(CH3)3C and (CH3)2CH] *ChemistrySelect*, **2017**, 2, 2021-2027	1.8	
7	Photoelectron Spectroscopy and Ionic Fragmentation of OSeCl2 and Its Analogue OSCl2 under VUV Irradiation. *Journal of Physical Chemistry A*, **2015**, 119, 8000-9	2.8	
6	Electronic properties and photofragmentation mechanisms of pyrosulfuryl chloride, ClSO2OSO2Cl. *Journal of Photochemistry and Photobiology A: Chemistry*, **2016**, 324, 184-191	4.7	
5	Comment on Molecular Structure analysis and Spectroscopic Characterization of Carbimazole with experimental (FT-IR, FT-Raman and UV–Vis) techniques and quantum chemical calculations [J. Mol. Struct. 1052 (2013) 38–49]. *Journal of Molecular Structure*, **2014**, 1056-1057, 216-218	3.4	
4	Crystal structure and spectroscopic properties of N?-methoxycarbonylsulfenyl-substituted ureas, CH3OC(O)SN(H)C(O)NRR? [R=H, R?=C(CH3)3 and R=R?=CH2CH3]. *Journal of Molecular Structure*, **2013**, 1037, 116-121	3.4	

3	COMPUTATIONAL INVESTIGATIONS, HIRSHFELD SURFACE ANALYSIS, INTERACTION ENERGY CALCULATIONS, AND ENERGY FRAMEWORK CRYSTAL STRUCTURE OF METHYL 2-AMINO-5-HYDROXYBENZOATE. *Journal of Structural Chemistry*, **2021**, 62, 1745-1758	0.9
2	Spectroscopic and thermal properties of stannadithiane compounds bearing endocyclic ether and lactone groups. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 210, 222-229	4.4
1	Preparation, structure determination, and in silico and in vitro Elastase inhibitory properties of substituted N-([1,1?-Biphenyl]-2-ylcarbamothioyl)- Aryl/Alkyl benzamide Derivatives. *Journal of Molecular Structure*, **2021**, 1245, 130993	3.4