

# CITATION REPORT

List of articles citing

Towards quantitative analysis of intermolecular interactions with Hirshfeld surfaces

DOI: 10.1039/b704980c

Chemical Communications, 2007, , 3814-6.

**Source:** <https://exaly.com/paper-pdf/42119178/citation-report.pdf>

**Version:** 2024-04-28

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
2288	Pressure-freezing with conformational conversion of 3-aminopropan-1-ol molecules. <b>2008</b> , 64, 476-82		4
2287	High-pressure structural study of L-alpha-glutamine and the use of Hirshfeld surfaces and graph-set notation to investigate the hydrogen bonding present in the structure up to 4.9 GPa. <b>2008</b> , 64, 466-75		15
2286	Hirshfeld Surfaces Identify Inadequacies in Computations of Intermolecular Interactions in Crystals: Pentamorphic 1,8-Dihydroxyanthraquinone. <b>2008</b> , 8, 4517-4525		389
2285	Polymorphism in 3-methyl-4-methoxy-4'-nitrostilbene (MMONS), a highly active NLO material. <b>2008</b> , 10, 197-206		42
2284	High-pressure polymorphism in amino acids. <b>2008</b> , 14, 143-184		103
2283	Isostructural relations in dihalomethanes and disproportionation of bromiodomethane. <b>2008</b> , 10, 1436		15
2282	Colored Polymorphs: Thermochemical and Structural Features of N-Picryl- p-toluidine Polymorphs and Solvates. <b>2008</b> , 8, 1977-1989		36
2281	Interactions in bisamide ionic liquids: Insights from a Hirshfeld surface analysis of their crystalline states. <b>2008</b> , 32, 2121		36
2280	Mapping Out the Molecular Interplay in Monohalobenzene Inclusion Complexes of p-H-calix[5]arene Using Hirshfeld Surfaces. <b>2008</b> , 8, 890-896		29
2279	Importance of Weak Hydrogen Bonds in the Formation of Cholamide Inclusion Crystals with Aromatic Guests. <b>2008</b> , 8, 1013-1022		28
2278	Kinetics of Desolvation and Structure of Bulky Xanthenol Inclusion Compounds. <b>2009</b> , 39, 163-168		3
2277	Crystal Structure of D,L-4-amino-(4-hydroxyphenyl)acetate, the Zwitter Ionic Form of Biologically Active D,L-4-hydroxyphenylglycine. <b>2009</b> , 39, 539-543		2
2276	Phosphine-free Sonogashira coupling: reactions of aryl halides catalysed by palladium(II) complexes of azetidine-derived polyamines under mild conditions. <b>2009</b> , 65, 1630-1634		28
2275	Solid state stacked trimers of 1,10-phenanthroline in a supramolecular tubular motif of C-methyl calix[4]resorcinarene. <b>2009</b> , 918, 10-13		3
2274	Hirshfeld surface analysis. <b>2009</b> , 11, 19-32		3999
2273	Highly fluoros complexes of ruthenium and osmium and their solubility in supercritical carbon dioxide. <b>2009</b> , 48, 11832-42		12
2272	Effects of weak intermolecular interactions on the molecular isomerism of tricobalt metal chains. <b>2009</b> , 131, 7580-91		25

2271	Functionalised azetidines as ligands: pyridyl-complemented coordination. <b>2009</b> , 434-42	13
2270	Exploring an Anti-Crystal Engineering Approach to the Preparation of Pharmaceutically Active Ionic Liquids. <b>2009</b> , 9, 1137-1145	104
2269	Enclathration by a xanthenol host via solid-solid reactions: structures and kinetics. <b>2009</b> , 33, 1960	4
2268	Electrostatic matching versus close-packing molecular arrangement in compressed dimethyl sulfoxide (DMSO) polymorphs. <b>2009</b> , 113, 2436-42	19
2267	Role of hydrogen bonding in the formation of glasses by small molecules: a triazine case study. <b>2009</b> , 19, 2747	35
2266	The effect of alkyl chain length in a series of novel N-alkyl-3-benzylimidazolium iodide salts. <b>2009</b> , 11, 2456	10
2265	Selectivity of butanol isomers by enclathration. <b>2009</b> , 11, 192-195	3
2264	Proton switching of polarity in metalloamphiphile crystals. <b>2009</b> , 11, 249-253	8
2263	Conformational and Synthron Polymorphism in Furosemide (Lasix). <b>2010</b> , 10, 1979-1989	113
2262	Layered Calcium Structures of p-Phosphonic Acid O-Methyl-Calix[6]arene. <b>2010</b> , 10, 3211-3217	14
2261	Mixed Ligand Palladium(II) Complex with NS-Bidentate S-Allyldithiocarbamate Schiff Base: Synthesis, Spectral Characterization, Crystal Structure and Decoding Intermolecular Interactions with Hirshfeld Surface Analysis. <b>2010</b> , 28, 221-228	21
2260	Crystal structure of dicyclopentadienylaluminum complex directed by weak C-H... interactions. <b>2010</b> , 968, 93-98	9
2259	N-H...N(pyridyl) and N-H...O(urea) hydrogen bonding and molecular conformation of N-aryl-N'-pyridylureas. <b>2010</b> , 968, 99-107	10
2258	Interplay of O-H...O, C-H...O and carbonyl...carbonyl interactions in crystal structures of o-benzoyl-l-tartaric acid and its anhydride. <b>2010</b> , 984, 75-82	11
2257	Pressure-induced phase transitions in L-alanine, revisited. <b>2010</b> , 66, 458-71	65
2256	Exceptionally large positive and negative anisotropic thermal expansion of an organic crystalline material. <b>2010</b> , 9, 36-9	204
2255	Solvatomorphism of 2-(4-Fluorophenylamino)-5-(2,4-dihydroxybenzeno)-1,3,4-thiadiazole Chloride. <b>2010</b> , 10, 3480-3488	29
2254	Experimental and Theoretical Charge Density Analysis of Polymorphic Structures: The Case of Coumarin 314 Dye. <b>2010</b> , 10, 1516-1526	32

2253	Reversible single-crystal to single-crystal polymorphic phase transformation of an organic crystal. <i>Chemical Communications</i> , <b>2010</b> , 46, 1676-8	5.8	37
2252	The thermosalient phenomenon. "Jumping crystals" and crystal chemistry of the anticholinergic agent oxitropium bromide. <b>2010</b> , 132, 14191-202		138
2251	Hydrogen bonded dimers vs. one-dimensional chains in 2-thiooxoimidazolidin-4-one (thiohydantoin) drug derivatives. <b>2010</b> , 12, 1730		13
2250	The $\beta$ and $\beta'$ forms of oxalic acid di-hydrate at high pressure: a theoretical simulation and a neutron diffraction study. <b>2010</b> , 12, 2596		22
2249	The Brønsted-Lowry Reaction Revisited: Glass-Forming Properties of Salts of 1,5-Dimethylbiguanide. <b>2010</b> , 10, 2734-2745		4
2248	Topochemistry and photomechanical effects in crystals of green fluorescent protein-like chromophores: effects of hydrogen bonding and crystal packing. <b>2010</b> , 132, 5845-57		141
2247	Three new co-crystals of hydroquinone: crystal structures and Hirshfeld surface analysis of intermolecular interactions. <b>2010</b> , 34, 193-199		236
2246	Relevance of weak hydrogen bonds in the conformation of organic compounds and bioconjugates: evidence from recent experimental data and high-level ab initio MO calculations. <b>2010</b> , 110, 6049-76		488
2245	Low temperature/high pressure polymorphism in DL-cysteine. <b>2010</b> , 12, 2551		44
2244	Self-assembly into infinite tapes by 2,7-disubstituted-1,8-naphthyridines in the solid state. <b>2010</b> , 12, 4074-4079		5
2243	Calixarene C8-imidazolium interplay as a design strategy for penetrating organic bi-layers. <b>2010</b> , 12, 573-578		28
2242	Solid State Transformations in Crystalline Salts. <b>2010</b> , 219-233		
2241	Investigation of sublimation with and without dissociation in the chloride and nitrate salts of 4-(1-hydroxy-1,2-diphenylethyl)pyridine. <b>2010</b> , 34, 405-413		3
2240	Horning-crown diamine complexes and salts: proton transfer mediated by solid-state intermolecular hydrogen bonding. <b>2011</b> , 13, 167-176		2
2239	Novel form V of tolbutamide and a high Z' crystal structure of form III. <b>2011</b> , 13, 47-51		33
2238	Supramolecular architectures in o-carboranyl alcohols bearing N-aromatic rings: syntheses, crystal structures and melting points correlation. <b>2011</b> , 13, 5788		30
2237	Pressure-induced pseudorotation in crystalline pyrrolidine. <b>2011</b> , 13, 15428-31		16
2236	Highly fluoros complexes of nickel, palladium and platinum: solubility and catalysis in high pressure CO <sub>2</sub> . <b>2011</b> , 40, 4167-74		8

2235	Tuning of spin crossover behaviour in iron(III) complexes involving pentadentate Schiff bases and pseudohalides. <b>2011</b> , 40, 10090-9	40
2234	Solid-State Forms of Resorcylic Acid: How Exhaustive Should a Polymorph Screen Be?. <b>2011</b> , 11, 210-220	49
2233	Cooperativity in Solid-State Squaramides. <b>2011</b> , 11, 3725-3730	12
2232	Supramolecular Self-Assembly of M-IDA Complexes Involving Lone-Pair $\cdots$ Interactions: Crystal Structures, Hirshfeld Surface Analysis, and DFT Calculations [H <sub>2</sub> IDA = iminodiacetic acid, M = Cu(II), Ni(II)]. <b>2011</b> , 11, 3250-3265	257
2231	Crystal Structure of Methyl Paraben Polymorph II. <b>2011</b> , 11, 967-971	18
2230	Insight into supramolecular self-assembly directed by weak interactions in acetophenone derivatives: crystal structures and Hirshfeld surface analyses. <b>2011</b> , 13, 6728	139
2229	Structural Extension from an Isonicotinic Acid Dimer to 4-(4-Pyridyl)benzoic Acid (pybenH) Dimer: X-ray Crystal Structure Analysis and Inclusion Properties of a Hydrogen-Bonded Coordination Polymer [Ni(SCN) <sub>2</sub> (pybenH) <sub>2</sub> ]. <b>2011</b> , 11, 5574-5591	11
2228	Charge Densities and Crystal Engineering. <b>2011</b> , 553-572	1
2227	Neutral and Zwitterionic Polymorphs of 2-(p-Tolylamino)nicotinic Acid. <b>2011</b> , 11, 4594-4605	24
2226	Use of Forces to steer the assembly of chromone derivatives into hydrogen bonded supramolecular layers: crystal structures and Hirshfeld surface analyses. <b>2011</b> , 13, 4528	186
2225	Cucurbit[n]urils (n = 5-8): A Comprehensive Solid State Study. <b>2011</b> , 11, 5598-5614	125
2224	On the Possibility of Tuning Molecular Edges To Direct Supramolecular Self-Assembly in Coumarin Derivatives through Cooperative Weak Forces: Crystallographic and Hirshfeld Surface Analyses. <b>2011</b> , 11, 4837-4849	165
2223	Multifunctional p-phosphonated calixarenes. <i>Chemical Communications</i> , <b>2011</b> , 47, 9764-72	5.8 44
2222	Halogen Bonding in 2,5-Dichloro-1,4-benzoquinone: Insights from Experimental and Theoretical Charge Density Analysis. <b>2011</b> , 11, 1855-1862	57
2221	Thione vs. ketone: The influence of the chalcogenide on weak intermolecular interactions in crystal packing of 4,5-bis(bromomethyl)-1,3-dithiole-2-thione and 4,5-bis(bromomethyl)-1,3-dithiol-2-one. <b>2011</b> , 1004, 296-302	2
2220	The CH $\cdots$ Hydrogen bond in chemistry. Conformation, supramolecules, optical resolution and interactions involving carbohydrates. <b>2011</b> , 13, 13873-900	644
2219	Acenes vs N-Heteroacenes: The Effect of N-Substitution on the Structural Features of Crystals of Polycyclic Aromatic Hydrocarbons. <b>2011</b> , 11, 5628-5633	40
2218	Enantiomeric crystallization of (-)-trans-1,2-diaminocyclohexane under pressure. <b>2011</b> , 13, 6742	13

2217	Amination-reduction reaction as simple protocol for potential boronic molecular receptors. Insight in supramolecular structure directed by weak interactions. <b>2011</b> , 9, 199-205	18
2216	A dinuclear oxo-bridged Fe(III) complex with tris(2-pyridylmethyl) amine: Structure and Hirshfeld surface analysis. <b>2011</b> , 994, 109-116	13
2215	Structural analysis and multipole modelling of quercetin monohydrate--a quantitative and comparative study. <b>2011</b> , 67, 63-78	61
2214	Experimental and theoretical electron-density study of three isoindole derivatives: topological and Hirshfeld surface analysis of weak intermolecular interactions. <b>2011</b> , 67, 569-81	27
2213	Synthesis and Theoretical Hirshfeld Analysis of a Supramolecular Heteropolyoxovanadate Architecture. <b>2011</b> , 2011, 1719-1724	19
2212	Can Hydrophobic Interactions Influence Supramolecular Aggregation in Self-Assembled Organic/Inorganic Hybrid Structures?. <b>2011</b> , 2011, 5125-5131	8
2211	The Solid-State Structures of Dimethylzinc and Diethylzinc. <b>2011</b> , 123, 11889-11891	11
2210	The solid-state structures of dimethylzinc and diethylzinc. <b>2011</b> , 50, 11685-7	38
2209	Macrocyclic multicenter complexes of nickel and copper of increasing complexity. <b>2011</b> , 17, 12385-95	6
2208	Structural elucidation and electronic properties of two pyrazole derivatives: A combined X-ray, Hirshfeld surface analyses and quantum mechanical study. <b>2011</b> , 506, 309-314	74
2207	Hydrogen bonding chains and rings structural motifs in new series of N-phthaloyl aminocarboxylic acid derivatives. Solid state microwave synthesis, structural chemistry, computational calculations and antimicrobial activity. <b>2011</b> , 994, 269-275	2
2206	Structural elucidation, Hirshfeld surface analysis and quantum mechanical study of para-nitro benzylidene methyl arjunolate. <b>2011</b> , 1000, 120-126	80
2205	A new parameter for classification of polycyclic aromatic hydrocarbon crystalline motifs: a Hirshfeld surface investigation. <b>2011</b> , 13, 7216	27
2204	Simulated pressure response of crystalline indole. <b>2011</b> , 135, 164508	15
2203	Factors Controlling Asymmetrization of the Simplest Linear I3 <sup>-</sup> and I4 <sup>2-</sup> Polyiodides with Implications for the Nature of Halogen Bonding. <b>2012</b> , 12, 1762-1771	41
2202	Inducing polarity in [VO3] <sup>3-</sup> chain compounds using asymmetric hydrogen-bonding networks. <b>2012</b> , 195, 86-93	13
2201	Seemingly simple group 8 cyclopentadienyl dicarbonyl metal halides: From little things, interesting things grow. <b>2012</b> , 14, 812-818	3
2200	Binding discrepancy of fluoride in quaternary ammonium and alkali salts by a tris(amide) receptor in solid and solution states. <b>2012</b> , 14, 5305	17

2199	Sodium ion association via bridging water molecules for different charged p-phosphonated calix[4]arene bilayers. <b>2012</b> , 14, 8541	3
2198	Computational study of methyl group dynamics in the hydroquinone clathrate of acetonitrile. <b>2012</b> , 14, 1570-2	9
2197	A cocrystal strategy for the precipitation of liquid 2,3-dimethyl pyrazine with hydroxyl substituted benzoic acid and a Hirshfeld surfaces analysis of them. <b>2012</b> , 14, 6860	54
2196	Conformational Flexibility and Cation-Anion Interactions in 1-Butyl-2,3-dimethylimidazolium Salts. <b>2012</b> , 12, 1838-1846	15
2195	Isomorphous Crystals by Chloro-Methyl Exchange in Polymorphic Fuchsones. <b>2012</b> , 12, 5411-5425	39
2194	Experimental and theoretical charge density study of the chemical bonding in chlorokojic acid crystal structure. <b>2012</b> , 116, 9759-68	8
2193	Quantifying intermolecular interaction of anthrylidene methyl arjunolate: Insights from Hirshfeld surface analysis. <b>2012</b> , 1021, 89-94	7
2192	Central-atom size effects on the methyl torsions of Group XIV tetratolyls. <b>2012</b> , 18, 13018-24	5
2191	Halogen Interactions in 2,4,5-Tribromoimidazolium Salts. <b>2012</b> , 2, 1017-1033	7
2190	Resolved structures of two picolinamide polymorphs. Investigation of the dimorphic system behaviour under conditions relevant to co-crystal synthesis. <b>2012</b> , 14, 8649	15
2189	Cobalt(II) scorpionate-like complexes obtained from in situ synthesized ligand created in [Co(0)-hydroxymethyl-3,5-dimethylpyrazole-VOSO <sub>4</sub> -NH <sub>4</sub> SCN] system. <b>2012</b> , 47, 104-111	23
2188	New Polymorphs of Fluconazole: Results from Cocrystallization Experiments. <b>2012</b> , 12, 240-252	44
2187	High-pressure spin-crossover in a dinuclear Fe(II) complex. <b>2012</b> , 14, 5265-71	63
2186	X-ray crystal structure of new monohydrate of 2-thioxoimidazolidin-4-one derivative and structural comparison with its analogs; visualizing intermolecular interactions with Hirshfeld surface analysis. <b>2012</b> , 23, 1559-1566	2
2185	Rubrene Polymorphs and Derivatives: The Effect of Chemical Modification on the Crystal Structure. <b>2012</b> , 12, 6035-6041	40
2184	Competition between the two-point and three-point synthon in cytosine-carboxylic acid complexes. <b>2012</b> , 14, 7065	17
2183	Amidothiourea as a potential receptor for organic bases by resonance assisted low barrier hydrogen bond formation: Structure and Hirshfeld surface analysis. <b>2012</b> , 14, 3306	6
2182	Guest Controlled Packing in Inclusion Compounds. <b>2012</b> , 42, 1014-1021	1

2181	Probing the relationships between molecular conformation and intermolecular contacts in N,N-dibenzyl-N'-(furan-2-carbonyl)thiourea. <b>2012</b> , 68, o19-22	15
2180	Phase transition between cubic and monoclinic polymorphs of the tetracyanoethylene crystal: the role of temperature and kinetics. <b>2012</b> , 14, 4656	19
2179	Dampened circumrotation by CH <sup>π</sup> interactions in hydrogen bonded [2]rotaxanes. <i>Chemical Communications</i> , <b>2012</b> , 48, 5677-9	5.8 25
2178	Are meloxicam dimers really the structure-forming units in the meloxicam-carboxylic acid co-crystals family? Relation between crystal structures and dissolution behaviour. <b>2012</b> , 14, 305-313	26
2177	A simple and robust method for the identification of packing motifs of aromatic compounds. <b>2012</b> , 14, 300-304	71
2176	Conformational Polymorphism in a Non-steroidal Anti-inflammatory Drug, Mefenamic Acid. <b>2012</b> , 12, 4283-4289	66
2175	Structural Versatility of Pyrene-2-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolane) and Pyrene-2,7-bis(4,4,5,5-tetramethyl-[1,3,2]dioxaborolane). <b>2012</b> , 12, 2794-2802	24
2174	Alkyl-Hauptgruppenmetall-Verbindungen: einfache Formeln, komplexe Strukturen. <b>2012</b> , 124, 1336-1337	
2173	Crystal packing in the 2-R,4-oxo-[1,3-a/b]-naphthodioxanes [Hirshfeld surface analysis and melting point correlation. <b>2012</b> , 14, 1083-1093	38
2172	Anion induced formation of supramolecular associations involving lone pair-π and anion-π interactions in Co(II) malonate complexes: experimental observations, Hirshfeld surface analyses and DFT studies. <b>2012</b> , 51, 3557-71	172
2171	Synthesis, Crystal Structure and Hirshfeld Surface Analysis of [Cu(EDTB)][CdBr <sub>4</sub> ]·H <sub>2</sub> O (EDTB = N,N,N',N'-tetrakis-(2-benzimidazolyl)methyl]-1,2-ethanediamine). <b>2012</b> , 42, 621-627	1
2170	Two-step postsynthetic modifications of a dinuclear Zn(II) coordination compound: Investigating the stability of the coordination chromophore. <b>2012</b> , 388, 135-139	10
2169	Short hydrogen bonds in a new salt of pyromellitic acid: An experimental charge density investigation. <b>2012</b> , 1014, 102-109	10
2168	Secondary interactions in the crystal structures of three 1,2,4,5-tetrakis(bromomethyl)-3,6-bis(2-alkoxy)benzenes. <b>2012</b> , 1016, 109-117	2
2167	Interplay of carbonyl-carbonyl, CH <sup>π</sup> O and CH <sup>π</sup> interactions in hierarchical supramolecular assembly of tartaric anhydrides [Tartaric acid and its O-acyl derivatives: Part 11. <b>2012</b> , 1017, 98-105	9
2166	Chiral crystals from an achiral molecule: 4,6-di-O-benzyl-1,3-O-benzylidene-2-O-(4-methoxybenzyl)-myo-5-inosose. <b>2012</b> , 68, o183-7	1
2165	Voronoi-Dirichlet tessellation as a tool for investigation of polymorphism in molecular crystals with C <sub>w</sub> H <sub>x</sub> N <sub>y</sub> O <sub>z</sub> composition and photochromic properties. <b>2012</b> , 68, 305-12	40
2164	X-ray diffraction and Raman study of DL-alanine at high pressure: revision of phase transitions. <b>2012</b> , 68, 412-23	25



2163	Main-group metal-alkyls: simple formulae but complex structural chemistry. <b>2012</b> , 51, 1310-1	2
2162	The interaction between theory and experiment in charge density analysis. <b>2013</b> , 87, 048104	5
2161	Strong intermolecular interactions shaping a small piano-stool complex. <b>2013</b> , 52, 10365-9	10
2160	Kinematic and mechanical profile of the self-actuation of thermosalient crystal twins of 1,2,4,5-tetrabromobenzene: a molecular crystalline analogue of a bimetallic strip. <b>2013</b> , 135, 13843-50	122
2159	A successive layer-by-layer assembly of supramolecular frameworks driven by a novel type of face-to-face $\pi\pi$ interactions. <b>2013</b> , 15, 7879	106
2158	Understanding the structure and electronic properties of molecular crystals under pressure: application of dispersion corrected DFT to oligoacenes. <b>2013</b> , 117, 8323-31	52
2157	Structural studies and physicochemical properties of L-valine hydrochloride monohydrate. <b>2013</b> , 15, 7372	36
2156	Steric-Induced Layer Flexion in Templated Vanadium Tellurites. <b>2013</b> , 13, 2190-2197	11
2155	Complexation of different metals with a novel N-donor bridging receptor and Hirshfeld surfaces analysis. <b>2013</b> , 397, 1-9	51
2154	Experimental and theoretical charge density analysis of a bromoethyl sulfonium salt. <b>2013</b> , 117, 14267-75	8
2153	Temperature Dependent Crystal Structure Analyses and Ion Volume Determinations of Organic Salts. <b>2013</b> , 639, 2153-2161	14
2152	Importance of O $\cdots$ N interaction between nitro groups in crystals. <b>2013</b> , 15, 10427	43
2151	Cobalt(II) complex containing two-ring scorpionate-like ligands formed in situ. Studies on the [Co(II)-hydroxymethyl-3,5-dimethylpyrazole-MoO <sub>3</sub> (H <sub>4</sub> I)] system. <b>2013</b> , 35, 22-26	14
2150	Heteroleptic (2-fluoro-3-pyridyl)arylboronic 8-oxyquinolines for the potential application in organic light-emitting devices. <b>2013</b> , 52, 10846-59	23
2149	Weak hydrogen bonds formed by thiol groups in N-acetyl-(L)-cysteine and their response to the crystal structure distortion on increasing pressure. <b>2013</b> , 117, 14247-60	22
2148	Weak C-H $\cdots$ O and Dipole-Dipole Interactions as Driving Forces in Crystals of Fluorosubstituted Phenylboronic Catechol Esters. <b>2013</b> , 13, 5344-5352	28
2147	Pholcodine monohydrate: Crystal structure and polymorphism. <b>2013</b> , 375, 119-124	1
2146	An investigation into the substituent effect of halogen atoms on the crystal structures of indole-3-carboxylic acid (ICA). <b>2013</b> , 15, 7490	27

2145	Tuning the formation of MOFs by pH influence: X-ray structural variations and Hirshfeld surface analyses of 2-amino-5-nitropyridine with cadmium chloride. <b>2013</b> , 15, 1772	172
2144	Systematic structural analysis of a series of anion receptor complexes. <b>2013</b> , 15, 9003	14
2143	MIIIMalonate Complexes (M = Mg, Cu, Ni and Co) Characterized by Layered Structures: Experimental Observation, Hirshfeld Surface Analysis and Theoretical Study. <b>2013</b> , 2013, 4679-4685	48
2142	Head-to-tail polymeric columnar structure of calix[4]arene possessing catechol arms in the solid state. <b>2013</b> , 15, 8404	5
2141	True and quasi-isomorphism in tetrakis(acetonitrile)coinage metal(I) salts. <b>2013</b> , 15, 1125	6
2140	Near-infrared pigments based on ion-pair charge transfer salts of dicationic and dianionic metal-dithiolene [M(II) = Pd, Pt] complexes. <b>2013</b> , 42, 12429-39	10
2139	Salt-bridge[and]interactions at work: associative interactions of sb[and]anion[and]n Cu(II)-malonate[and]2-aminopyridine[and]hexafluoridophosphate ternary system. <b>2013</b> , 15, 686-696	51
2138	Intermolecular friction symbol derived from crystal information. <b>2013</b> , 15, 6837	57
2137	Four Polymorphs of Methyl Paraben: Structural Relationships and Relative Energy Differences. <b>2013</b> , 13, 1206-1217	37
2136	Pressure versus temperature effects on intramolecular electron transfer in mixed-valence complexes. <b>2013</b> , 19, 195-205	12
2135	Superacidic or not? Synthesis, characterisation, and acidity of the room-temperature ionic liquid [C(CH <sub>3</sub> ) <sub>3</sub> ] <sup>+</sup> [Al <sub>2</sub> Br <sub>7</sub> ] <sup>-</sup> . <b>2013</b> , 19, 109-16	27
2134	Synthesis and structural study of N-acetyl-1,2,3,4-tetrahydroisoquinoline-2-sulfonamide obtained using H <sub>6</sub> P <sub>2</sub> W <sub>18</sub> O <sub>62</sub> as acidic solid catalyst. <b>2013</b> , 1041, 6-15	7
2133	Supramolecular chirality-sensing DNA-mimicry of a norbornane derivative decorated with isoxazoline and methylpyrrolidine-2,5-dione ring. <b>2013</b> , 1041, 164-174	3
2132	Influence of the ortho-methoxyalkyl substituent on the properties of phenylboronic acids. <b>2013</b> , 1035, 190-197	12
2131	Unique Type II Halogen[and]Halogen Interactions in Pentafluorophenyl-Appended 2,2'-Bithiazoles. <b>2013</b> , 13, 1045-1049	43
2130	On polymorphism of 2-(4-fluorophenylamino)-5-(2,4-dihydroxybenzeno)-1,3,4-thiadiazole (FABT) DMSO solvates. <b>2013</b> , 15, 1978	27
2129	Quantitative crystal structure analysis of 1,3,4-thiadiazole derivatives. <b>2013</b> , 15, 4549	40
2128	Tuning solid-state fluorescence of pyrene derivatives via a cocrystal strategy. <b>2013</b> , 15, 3623	58

2127	Structural Study of Prolinium/Fumaric Acid Zwitterionic Cocrystals: Focus on Hydrogen-Bonding Pattern Involving Zwitterionic (Ionic) Heterosynthons. <b>2013</b> , 13, 2373-2389	16
2126	Aryl-substituents moderate the nature of hydrogen bonds, N $\cdots$ N versus N $\cdots$ O, leading to supramolecular chains in the crystal structures of N-arylamino 1,2,3-triazole esters. <b>2013</b> , 15, 4917	36
2125	Polymorphism in metformin embonate salt –recurrence of dimeric and tetrameric guanidinium-carboxylate synthons. <b>2013</b> , 15, 4448	18
2124	Exploring contribution of intermolecular interactions in supramolecular layered assembly of naphthyridine co-crystals: Insights from Hirshfeld surface analysis of their crystalline states. <b>2013</b> , 1048, 157-165	32
2123	Crystal Structures and Density Functional Theory Calculations of o- and p-Nitroaniline Derivatives: Combined Effect of Hydrogen Bonding and Aromatic Interactions on Dimerization Energy. <b>2013</b> , 13, 3603-3612	15
2122	The effects of P $\cdots$ changes on intermolecular interactions in crystal structure of iodoform. <b>2013</b> , 1041, 106-112	9
2121	Crystal structure, vibrational and theoretical studies of bis(1,4-H $_2$ -1,2,4-triazolium) hexachloridostannate(IV) monohydrate. <b>2013</b> , 1032, 56-61	23
2120	Molecules in crystals. <b>2013</b> , 87, 048103	101
2119	Chemical bond characterization of a mixed-valence tri-cobalt complex, Co $_3$ (Edmtrz) $_4$ (EOH) $_2$ (CN) $_6$ ·2H $_2$ O. <b>2013</b> , 52, 11023-33	12
2118	Two Novel Salts of Tris(hydroxymethyl)aminomethane (THAM): Synthesis, Crystal Structure, Thermal and Hirshfeld Surfaces Analysis. <b>2013</b> , 43, 576-584	8
2117	Lewis acidity and sugar receptor activity of 3-amino-substituted benzoxaboroles and their ortho-aminomethylphenylboronic acid analogues. <b>2013</b> , 37, 188-194	35
2116	Hirshfeld surface analysis of new phosphoramidates. <b>2013</b> , 69, 260-70	26
2115	Synthesis, crystal structure, Hirshfeld surfaces, and spectral properties of Cu(II) and Co(II) complexes with 3-phenoxyethyl-4-phenyl-5-(2-pyridyl)-1,2,4-triazole. <b>2013</b> , 66, 3100-3112	21
2114	Exploring supramolecular self-assembly of tetraarylporphyrins by halogen bonding: crystal engineering with diversely functionalized six-coordinate tin(II)-porphyrin tectons. <b>2013</b> , 19, 14941-9	36
2113	An FeII Spin-Crossover Complex Becomes Increasingly Cooperative with Ageing. <b>2013</b> , 2013, 745-752	14
2112	Ein kleiner Klavierstuhl-Komplex, geformt durch starke intermolekulare Wechselwirkungen. <b>2013</b> , 125, 10555-10559	9
2111	Solid state assembly of cyclic $\beta$ -peptoids. <b>2014</b> , 16, 3667-3687	47
2110	Effect of high pressure on the crystal structure and charge transport properties of the (2-fluoro-3-pyridyl)(4-iodophenyl)borinic 8-oxyquinolate complex. <b>2014</b> , 16, 10780-10790	8

2109	Towards the chemical control of molecular packing: syntheses and crystal structures of three trans-[NiL <sub>4</sub> (NCS) <sub>2</sub> ] complexes. <b>2014</b> , 70, 115-25	13
2108	The enrichment ratio of atomic contacts in crystals, an indicator derived from the Hirshfeld surface analysis. <b>2014</b> , 1, 119-28	258
2107	Influences of halogen atoms on indole-3-acetonitrile (IAN): Crystal structure and Hirshfeld surfaces analysis. <b>2014</b> , 1076, 679-686	8
2106	What difference does a methyl group make: pentamethylbenzene?. <b>2014</b> , 15, 3776-81	6
2105	Tin and Mercury Compounds Supported by a Bulky Organometallic Ligand Incorporating a Pendant Guanidine Functionality. <b>2014</b> , 67, 1071	5
2104	Accurate and Efficient Model Energies for Exploring Intermolecular Interactions in Molecular Crystals. <b>2014</b> , 5, 4249-55	258
2103	3-Picoline mediated self-assembly of M(II)-malonate complexes (M = Ni/Co/Mn/Mg/Zn/Cu) assisted by various weak forces involving lone pair-π and anion-π interactions. <b>2014</b> , 118, 14713-26	77
2102	Polymorphs Related by an Enantiotropic Phase Transition but Having Only Order-Disorder-Level Conformational Differences in a Spiro-Conjugated Imidazolidine Ring Compound. <b>2014</b> , 14, 6302-6310	4
2101	Charge density analysis for crystal engineering. <b>2014</b> , 8, 68	34
2100	Structural elucidation and contribution of intermolecular interactions in O-hydroxy acyl aromatics: Insights from X-ray and Hirshfeld surface analysis. <b>2014</b> , 1064, 70-75	63
2099	Theoretical calculation and structural studies for a new nitrogen derivative from nor-lapachol. <b>2014</b> , 1060, 233-238	2
2098	A thermally labile copper (II) complex with hetero N- and O-donor ligands: crystal structure, Hirshfeld surfaces, thermal and luminescent properties. <b>2014</b> , 122, 246-51	3
2097	Dicyanamide mediated construction of 1D polymeric networks of quinoxaline with d <sup>10</sup> metal ions: Synthesis, thermogravimetric analysis, photoluminescence and a theoretical investigation on the π-π interactions. <b>2014</b> , 70, 11-19	17
2096	Polymorphism in Bulk and Thin Films: The Curious Case of Dithiophene-DPP(Boc)-Dithiophene. <b>2014</b> , 118, 657-669	26
2095	Molecular Imprisonment: Host Response to Guest Location, Orientation, and Dynamics in Clathrates of Dianin <sup>III</sup> Compound. <b>2014</b> , 14, 1296-1306	16
2094	Synthesis, structural characterization and DFT calculations of a new one-dimensional diorganotin(IV) derivative of N-isonicotinyl phosphoramidate. <b>2014</b> , 71, 8-16	18
2093	Crystal structure, Hirshfeld surfaces and DNA cleavage investigation of two copper(II) complexes containing polypyridine and salicylide ligands. <b>2014</b> , 126, 81-5	3
2092	Experimental Electron Density and Neutron Diffraction Studies on the Polymorphs of Sulfathiazole. <b>2014</b> , 14, 1227-1239	36

2091	On the Formation of Droperidol Solvates: Characterization of Structure and Properties. <b>2014</b> , 14, 2654-2664	53
2090	Intermolecular Interactions in Fluorinated Tetraarylporphyrins: An Experimental and Theoretical Study. <b>2014</b> , 2014, 2653-2662	26
2089	Polymorphism of cis-1,4-cyclohexanediol, a new plastic crystal former. Considerations on isomeric cyclohexanediols plastic crystal forming abilities. <b>2014</b> , 1078, 10-19	11
2088	The superacid HBr/AlBr <sub>3</sub> : protonation of benzene and ordered crystal structure of [C(6)H(7)] <sup>(+)</sup> [Al(2)Br(7)] <sup>(-)</sup> . <b>2014</b> , 53, 1689-92	20
2087	Exploration of supramolecular layer and bi-layer architecture in M(II)PPP complexes: Structural elucidation and Hirshfeld surface analysis [PPP = 4-(3-Phenylpropyl)pyridine, M = Cu(II), Ni(II)]. <b>2014</b> , 1070, 65-74	61
2086	A Donor-Acceptor-Donor Structured Organic Conductor with S <sup>⋯</sup> S Chalcogen Bonding. <b>2014</b> , 14, 459-466	50
2085	Die Supersäure HBr/AlBr <sub>3</sub> : Protonierung von Benzol und ausgeordnete Kristallstruktur von [C <sub>6</sub> H <sub>7</sub> ] <sup>+</sup> [Al <sub>2</sub> Br <sub>7</sub> ] <sup>-</sup> . <b>2014</b> , 126, 1715-1718	13
2084	Intermolecular interactions in solid-state metalloporphyrins and their impacts on crystal and molecular structures. <b>2014</b> , 53, 11552-62	7
2083	Hydrogen-Bonded Supramolecular Architectures Based on Tris(Hydranilato)Metallate(III) (M = Fe, Cr) Metallotectons. <b>2014</b> , 14, 5938-5948	19
2082	Synthesis, crystal structures and phase transformation of the new solid-state forms of tetrandrine. <b>2014</b> , 4, 62586-62593	17
2081	Crystallization in Ionic Liquids: Synthesis, Properties, and Polymorphs of Uranyl Salts. <b>2014</b> , 14, 6421-6432	16
2080	Tunable trimers: using temperature and pressure to control luminescent emission in gold(I) pyrazolate-based trimers. <b>2014</b> , 20, 16933-42	23
2079	Analysis of intermolecular interactions in 3-(4-fluoro-3-phenoxyphenyl)-1-((4-methylpiperazin-1-yl)methyl)-1H-1,2,4-triazole-5-thiol. <b>2014</b> , 126, 1337-1345	5
2078	Guest induced head-to-tail columnar assembly of 5,17-difunctionalized calix[4]arene. <b>2014</b> , 16, 6023-6032	8
2077	Hydrogen-Bonded Dimeric Synthon of Fluoro-Substituted Phenylboronic Acids versus Supramolecular Organization in Crystals. <b>2014</b> , 14, 5912-5921	23
2076	Simultaneous co-ordination of three cytosine ligands displaying different binding sites around the copper centres. <b>2014</b> , 4, 44938-44942	6
2075	Fine-tuning solid-state luminescence in NPIs (1,8-naphthalimides): impact of the molecular environment and cumulative interactions. <b>2014</b> , 16, 20866-77	27
2074	Porous molecular crystals by macrocyclic coordination supramolecules. <b>2014</b> , 136, 14883-95	41

- 2073 Vibrational spectra of the ortho-nitroanilinium cation in torsional space. Theoretical studies vs. experimental data of ortho-nitroanilinium chloride. **2014**, 132, 776-85 11
- 2072 Crystal Packing of Impact-Sensitive High-Energy Explosives. **2014**, 14, 6101-6114 133
- 2071 Exploring secondary bonding in p-block chemistry: An experimental study of [GeX<sub>2</sub>{o-C<sub>6</sub>H<sub>4</sub>(PMe<sub>2</sub>)<sub>2</sub>}] using variable pressure single crystal X-ray diffraction. **2014**, 16, 8169
- 2070 Ligand hierarchy on driving the crystal packing. Effect of supramolecular interactions on solid-state conformations adopted by saccharinate Pd(II) complexes. **2014**, 16, 7124 2
- 2069 Experimental and theoretical analysis of  $\pi$ - $\pi$  intermolecular interactions in derivatives of 1,2,4-triazoles. **2014**, 16, 1702-1713 51
- 2068 Boron Cluster Anions [B<sub>n</sub>H<sub>n</sub>]<sub>2</sub> (n = 10, 12) in Reactions of Iron(II) and Iron(III) Complexation with 2,2'-Bipyridyl and 1,10-Phenanthroline. **2014**, 640, 2149-2160 17
- 2067 Dual modes of binding on the hexafluorosilicate anion by a C<sub>3v</sub> symmetric flexible tripodal amide ligand in solid state. **2014**, 16, 4886-4891 13
- 2066 Polymorphism in two biologically active dihydropyrimidinium hydrochloride derivatives: quantitative inputs towards the energetics associated with crystal packing. **2014**, 70, 681-96 23
- 2065 Hirshfeld surface analysis of crystal packing in aza-aromatic picrate salts. **2014**, 16, 4508-4538 20
- 2064 Pressure-Induced Conformational Change in Organic Semiconductors: Triggering a Reversible Phase Transition in Rubrene. **2014**, 118, 13476-13483 28
- 2063 Computational Study of the Formation of Short Centrosymmetric N<sup>+</sup>H...S<sup>-</sup> Supramolecular Synthons and Related Weak Interactions in Crystalline 1,2,4-Triazoles. **2014**, 14, 5881-5896 23
- 2062 High-Throughput Investigation of the Geometry and Electronic Structures of Gas-Phase and Crystalline Polycyclic Aromatic Hydrocarbons. **2014**, 118, 19964-19974 19
- 2061 (NH<sub>4</sub>)<sub>4</sub>Sn<sub>2</sub>S<sub>6</sub>·3H<sub>2</sub>O: Crystal Structure, Thermal Decomposition, and Precursor for Textured Thin Film. **2014**, 26, 4494-4504 16
- 2060 Synthesis of the first morpholine-containing iron(II) clathrochelates: A new class of efficient functionalized transcription inhibitors. **2014**, 421, 300-306 15
- 2059 Crystal Packing of Low-Sensitivity and High-Energy Explosives. **2014**, 14, 4703-4713 211
- 2058 Melting point-solubility-structure correlations in multicomponent crystals containing fumaric or adipic acid. **2014**, 16, 9992-9998 33
- 2057 Evident Hydrogen Bonded Chains Building CL-20-Based Cocrystals. **2014**, 14, 3923-3928 46
- 2056 Crystal-to-Crystal Thermal Phase Transformation of Polymorphs of Isomeric 2,3-Naphthalene Diol Ditoluates: Mechanism and Implications for Molecular Crystal Formation and Melting. **2014**, 14, 4985-4996 10

2055	Tracing a Crystallization Pathway of an RT Liquid, 4-Fluorobenzoyl Chloride: Metastable Polytypic Form as an Intermediate Phase. <b>2014</b> , 14, 4230-4235	3
2054	Structural and spectroscopic characterization and Hirshfeld surface analysis of major component of antibiotic mupirocin [pseudomonic acid A. <b>2014</b> , 1076, 126-135	12
2053	A combined experimental and theoretical study of the supramolecular self-assembly of Cu(II) malonate complex assisted by various weak forces and water dimer. <b>2014</b> , 220, 149-156	19
2052	Polymorphism Arising from Differing Rates of Compression of Liquids. <b>2014</b> , 14, 3384-3391	20
2051	Polymorphic Signature of the Anti-inflammatory Activity of 2,2'-[[1,2-Phenylenebis(methylene)]bis(sulfanediyl)]bis(4,6-dimethylnicotinonitrile). <b>2014</b> , 14, 1347-1356	17
2050	Intermolecular Interactions and Second-Harmonic Generation Properties of (E)-1,5-Diarylpen-tenyn-1-ones. <b>2014</b> , 14, 4402-4410	16
2049	Two new complexes with 6-methylnicotinic acid ligand: Synthesis, crystal structure and Hirshfeld surfaces. <b>2014</b> , 412, 60-66	19
2048	Comparison of the structural motifs and packing arrangements of six novel derivatives and one polymorph of 2-(1-phenyl-1H-1,2,3-triazol-4-yl)pyridine. <b>2014</b> , 70, 379-89	9
2047	Subtle C <sup>δ</sup> ...Hal (Hal = Cl, Br) Bonding as Predominant Synthons in the Assembly of Supramolecular Architectures Based on Luminescent Tin(IV) Complexes. Crystallography, Hirshfeld Surfaces, DFT Calculations, and Fluorescence. <b>2014</b> , 14, 3742-3757	17
2046	Unusual hydrogen bond patterns contributing to supramolecular assembly: conformational study, Hirshfeld surface analysis and density functional calculations of a new steroid derivative. <b>2014</b> , 16, 7802-7814	14
2045	A structural framework of biologically active coumarin derivatives: crystal structure and Hirshfeld surface analysis. <b>2014</b> , 16, 6654-6663	19
2044	Discrete cubic water cluster: An unusual building block of 3D supramolecular network. <b>2014</b> , 43, 60-63	66
2043	Toward low-sensitive and high-energetic co-crystal II: structural, electronic and energetic features of CL-20 polymorphs and the observed CL-20-based energetic co-crystals. <b>2014</b> , 16, 5905	77
2042	Weak hydrogen bonds in bis(3-nitroanilinium) hexachloridostannate monohydrate. X-ray, vibrational and theoretical studies. <b>2014</b> , 131, 335-41	16
2041	In situ synthesis of scorpion-like complexes isolated from the system containing zerovalent nickel. <b>2014</b> , 78, 31-39	11
2040	Cooperativity of anion-π and π-π interactions regulates the self-assembly of a series of carbene proligands: Towards quantitative analysis of intermolecular interactions with Hirshfeld surface. <b>2014</b> , 1068, 58-70	38
2039	Fabrication of two supramolecular self-assemblies of Mn(II)-dicarboxylates with trans-4,4'-azobispyridine: Analysis of H-bonding interactions with Hirshfeld surfaces and DFT calculations. <b>2014</b> , 1067, 64-73	3
2038	The [Sn <sub>2</sub> S <sub>6</sub> ] <sup>4-</sup> Anion Acting as Tetradentate Linker: Solvothermal Synthesis and Selected Properties of [TM(phen) <sub>2</sub> ] <sub>2</sub> Sn <sub>2</sub> S <sub>6</sub> and [TM(phen) <sub>2</sub> ] <sub>2</sub> Sn <sub>2</sub> S <sub>6</sub> ·phen·H <sub>2</sub> O (TM = Fe, Co). <b>2014</b> , 640, 2858-2863	18

- 2037 Unusual Crystal Packing in a Family of [Fe{2,6-bis(pyrazol-3-yl)pyridine}2]2+ Compounds and the Effect on the Occurrence of Spin Crossover and Its Cooperative Character. **2014**, 2014, 6013-6021 17
- 2036 Crystallography of Ionic Liquids. **2015**, 231-534 3
- 2035 Second-Sphere Complexation of Thorium(IV) by Cucurbit[6]uril with Included Perrhenate Counterions [Crystal Structure and Hirshfeld Surface Analysis. **2015**, 2015, 2037-2040 7
- 2034 Bis(quinoxaline-dithiolato)nickel(III) Complexes [Bu4N][NiIII(6,7-qdt)2] and [Ph4P][NiIII(Ph26,7-qdt)2]·CHCl3 (6,7-qdt = Quin[boxaline-6,7-dithiolate; Ph26,7-qdt = Diphenylquinoxaline-6,7-dithiolate): Synthesis, Spectroscopy, Electrochemistry, DFT Calculations, Crystal Structures and Hirshfeld Surface Analysis. **2015**, 2015, 5523-5533 3
- 2033 Estimation of Lattice Enthalpies of Ionic Liquids Supported by Hirshfeld Analysis. **2015**, 16, 2890-2898 9
- 2032 Isoenergetic Polymorphism: The Puzzle of Tolazamide as a Case Study. **2015**, 21, 15395-404 20
- 2031 Experimental and Theoretical Charge Density Study on Di-2-pyrazylamine (Hdpza) Molecule in Crystal. **2015**, 62, 712-721 2
- 2030 Single-Crystal-to-Single-Crystal Transition in an Enantiopure [7]Helquat Salt: The First Observation of a Reversible Phase Transition in a Helicene-Like Compound. **2015**, 21, 13508-12 5
- 2029 Two Pseudopolymorphic Star-Shaped Tetranuclear Co(3+) Compounds with Disulfide Anions Exhibiting Two Different Connection Modes and Promising Photocatalytic Properties. **2015**, 21, 13637-45 4
- 2028 Exploration of CH $\pi$  Interactions involving the  $\pi$  System of pseudohalide coligands in metal complexes of a Schiff-base ligand. **2015**, 17, 4680-4690 71
- 2027 Experimental (X-ray, (13)C CP/MAS NMR, IR, RS, INS, THz) and Solid-State DFT Study on (1:1) Co-Crystal of Bromanilic Acid and 2,6-Dimethylpyrazine. **2015**, 119, 6852-72 14
- 2026 Structural characterization of LASSBio-1289: a new vasoactive N-methyl-N-acylhydrazone derivative. **2015**, 17, 165-173 10
- 2025 Resolution of malic acid by (+)-cinchonine and (–)-cinchonidine. **2015**, 93, 858-863
- 2024 On the relaxation dynamics in active pharmaceutical ingredients: solid-state 1H NMR, quasi-elastic neutron scattering and periodic DFT study of acebutolol hydrochloride. **2015**, 5, 57502-57514 3
- 2023 An experimental and computational investigations of supramolecular anion $\pi$  Anion assemblies in mononuclear Zn(II) complexes with a versatile tetradentate N-donor Schiff base ligand. **2015**, 102, 764-772 3
- 2022 Structural elucidation, density functional calculations and contribution of intermolecular interactions in cholest-4-en-3-one crystals: Insights from X-ray and Hirshfeld surface analysis. **2015**, 1084, 274-283 19
- 2021 Synthesis of electron-deficient fluorinated porphyrins through scrambling: Characterization and quantitative crystal structure analysis. **2015**, 170, 10-16 12
- 2020 Synthesis and structural elucidation of a novel polymorph of alcaftadine. **2015**, 142, 311-9 5



2019	The role of hydrogen bonding on supramolecular assembly of the mercury coordination compounds and final structure influenced by solvent effect. <b>2015</b> , 429, 1-14	16
2018	Concerted mitigation of O <sup>⋯</sup> H and C(=O) <sup>⋯</sup> H interactions prospects sixfold gain in optical nonlinearity of ionic stilbazolium derivatives. <b>2015</b> , 7, 4693-8	16
2017	Structural and ab initio studies on the polymorphism of iminophosphorane (CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> PNP[(O)(OPh) <sub>2</sub> ]. <b>2015</b> , 1083, 389-397	2
2016	Synthesis, characterization and crystal structure determination of Mn (II) ion based 1D polymer constructed from 2, 2' bipyridyl and azide group, its thermal stability, magnetic properties and Hirshfeld surface analysis. <b>2015</b> , 225, 249-255	12
2015	Molecular structure studies of (1,2)-2-benzyl-2,3-dihydro-2-(1H-inden-2-yl)-1H-inden-1-ol. <b>2015</b> , 1083, 286-299	8
2014	Tetramorphs of the Antibiotic Drug Trimethoprim: Characterization and Stability. <b>2015</b> , 15, 1745-1756	28
2013	Synthesis, Characterization and Hirshfeld Surface Analysis of a 2-thiophene Acetic Acid Derivative. <b>2015</b> , 607, 223-231	2
2012	One hydrogen bond does not a separation make, or does it? Resolution of amines by diacetoneketogulonic acid. <i>Chemical Communications</i> , <b>2015</b> , 51, 5664-7	5.8 3
2011	Polymorphism in anti-hyperammonemic agent N-carbamoyl-L-glutamic acid. <b>2015</b> , 17, 5252-5265	7
2010	Vinyl sulfone building blocks in covalently reversible reactions with thiols. <b>2015</b> , 39, 5841-5853	14
2009	Interlocked aromatic species: Crystal structure and Hirshfeld surface analysis of the uranyl ion complex of 3-(pyrimidin-2-yl)benzoate with Ni(phen) 3 2+ counter-ions. <b>2015</b> , 59, 25-27	10
2008	Location of Ge and extra-framework species in the zeolite ITQ-24. <b>2015</b> , 44, 6288-95	12
2007	Structural changes in MII dithione/dithiolato complexes (M = Ni, Pd, Pt) on varying the dithione functionalization. <b>2015</b> , 17, 4161-4171	5
2006	Structural, electrical, ferroelectric and mechanical properties with Hirshfeld surface analysis of novel NLO semiorganic sodium p-nitrophenolate dihydrate piezoelectric single crystal. <b>2015</b> , 5, 57735-57748	68
2005	A hexanuclear gold carbonyl cluster. <b>2015</b> , 6, 5506-5510	5
2004	New supramolecular cocrystal of 2-amino-5-chloropyridine with 3-methylbenzoic acids: Syntheses, structural characterization, Hirshfeld surfaces and quantum chemical investigations. <b>2015</b> , 1099, 246-256	50
2003	Halogen Bonding in Host-Guest Compounds: Structures and Kinetics of Enclathration and Desolvation. <b>2015</b> , 15, 3271-3279	18
2002	Isoquinoline-based Werner clathrates with xylene isomers: aromatic interactions vs. molecular flexibility. <b>2015</b> , 44, 6863-70	13

2001	Stereo-selective synthesis, structural and antibacterial studies of novel glycosylated 2,3-amino acid analogues. <b>2015</b> , 24, 3174-3193	3
2000	Understanding the packing in the 1 : 1 molecular complex 1,3,5-tricyanobenzene-hexamethylbenzene by probing lattice modes. <b>2015</b> , 17, 3787-3792	2
1999	New water soluble heterometallic complex showing unpredicted coordination modes of EDTA. <b>2015</b> , 230, 61-69	11
1998	Experimental and theoretical studies on the structure and spectroscopic properties of N-scorpionate complexes obtained from metallic cobalt in a one pot synthesis. <b>2015</b> , 95, 60-68	15
1997	Conformational Simulation of Sulfamethizole by Molecular Complexation and Insights from Charge Density Analysis: Role of Intramolecular S...O Chalcogen Bonding. <b>2015</b> , 15, 2110-2118	44
1996	Exploring Supramolecular Self-Assembly of Tetraarylporphyrins by Halogen Interactions. 3. Tin(L)2(A2B2-Porphyrin) Arrays Supported by Concerted Halogen and Hydrogen Bonding. <b>2015</b> , 15, 3063-3075 <sup>21</sup>	21
1995	Computationally Assisted (Solid-State Density Functional Theory) Structural (X-ray) and Vibrational Spectroscopy (FT-IR, FT-RS, TDs-THz) Characterization of the Cardiovascular Drug Lacidipine. <b>2015</b> , 15, 2817-2830	15
1994	Unusually short chalcogen bonds involving organoselenium: insights into the Se-N bond cleavage mechanism of the antioxidant ebselen and analogues. <b>2015</b> , 21, 6793-800	65
1993	Hirshfeld Surface Investigation of Structure-Directing Interactions within Dipicolinic Acid Derivatives. <b>2015</b> , 15, 1697-1706	55
1992	Structural Characterization and Rationalization of Formation, Stability, and Transformations of Benperidol Solvates. <b>2015</b> , 15, 2337-2351	36
1991	A charge density study of delocalization and intermolecular interactions. <b>2015</b> , 17, 14177-84	7
1990	Expanding the structural versatility of thioostannate(IV) complexes. <b>2015</b> , 17, 2413-2420	13
1989	Phosphoramides bearing isoxazole derivative: spectroscopic and structural characterization, study of hydrogen-bonding interactions and two lanthanide complexes (Ln(III) = Ce and Eu). <b>2015</b> , 71, 176-85	3
1988	Influence of substituents on cation-anion contacts in imidazolium perchlorates. <b>2015</b> , 44, 8669-77	8
1987	Synthesis, Characterization, Crystal Structure, and Hirshfeld Surface Analysis of (Z)-3-(methylsulfanyl)-2,3-diphenylprop-2-enenitrile. <b>2015</b> , 609, 140-154	3
1986	Solvent-controlled construction of manganese(II) complexes with 4-acetylpyridine nicotinoylhydrazone ligand. <b>2015</b> , 438, 220-231	8
1985	Contrasting Solid-State Fluorescence of Dienes with Small and Large Aryl Substituents: Crystal Packing Dependence and Stimuli-Responsive Fluorescence Switching. <b>2015</b> , 119, 10481-93	17
1984	New oxovanadium(IV) complexes with pincer ligand obtained in situ: experimental and theoretical studies on the structure, spectroscopic properties and antitumour activity. <b>2015</b> , 5, 85470-85479	14

1983	Exploration of Supramolecular Architecture in Complexes with 1-Substituted-1H-[1,2,3]-triazole-4-carboxylic Acid: Structural Elucidation and Hirshfeld Surface Analysis. <b>2015</b> , 25, 1233-1238	3
1982	Furosemide Cocrystals with Pyridines: An Interesting Case of Color Cocrystal Polymorphism. <b>2015</b> , 15, 5858-5872	32
1981	Rich synthetic and structural chemistry of polynuclear Pb(II)Cu(I)/Ag(I) heterobimetallic thiolate clusters, their decomposition and generation of a Cu(II) hydrosulfide variant. <b>2015</b> , 5, 94486-94494	5
1980	Nickel(II) complexes having Imidazol-2-ylidene-N <sup>2</sup> -phenylurea ligand in the coordination sphere □ syntheses and solid state structures. <b>2015</b> , 127, 1397-1404	0
1979	Significant Role of Supramolecular Interactions on Conformational Modulation of Flexible Organic Cation Receptors in a Metal-Bis(dithiolate) Coordination Complex Matrix. <b>2015</b> , 15, 4459-4474	5
1978	A strategy developed from the observed energeticenergetic cocrystals of BTF: cocrystallizing and stabilizing energetic hydrogen-free molecules with hydrogenous energetic cofomer molecules. <b>2015</b> , 17, 7150-7159	22
1977	Charge density and optical properties of multicomponent crystals containing active pharmaceutical ingredients or their analogues. <b>2015</b> , 71, 392-405	8
1976	Electron Density Distribution of Urea in Co-crystals with Rigid and Flexible Dicarboxylic Acids. <b>2015</b> , 15, 5578-5592	9
1975	Two new organotin(IV)-phosphoryl complexes: crystal structure and Hirshfeld surface analysis. <b>2015</b> , 12, 2093-2103	2
1974	Double helicity induction in chiral bis(triphenylacetamides). <b>2015</b> , 5, 83448-83458	12
1973	Hirshfeld surface analysis of two new phosphorothioic triamide structures. <b>2015</b> , 71, 824-33	2
1972	Tetrahedral Tetraphosphonic Acids. New Building Blocks in Supramolecular Chemistry. <b>2015</b> , 15, 4925-4931	19
1971	Organic alloys of room temperature liquids thiophenol and selenophenol. <i>Chemical Communications</i> , <b>2015</b> , 51, 14255-8	5.8 37
1970	Intermolecular interactions in crystalline 1-(adamantane-1-carbonyl)-3-substituted thioureas with Hirshfeld surface analysis. <b>2015</b> , 17, 7551-7563	59
1969	Hirshfeld surface analysis of sulfameter (polymorph III), sulfameter dioxane monosolvate and sulfameter tetrahydrofuran monosolvate, all at 296 K. <b>2015</b> , 71, 944-53	4
1968	Supramolecular Recognition and Energy Frameworks in HostGuest Complexes of 18-Crown-6 and Sulfonamides. <b>2015</b> , 15, 5892-5900	23
1967	X-ray, vibrational and theoretical studies of weak hydrogen bonds in bis(4-nitroanilinium) hexachloridostannate. <b>2015</b> , 139, 102-7	7
1966	Crystal Engineering and Charge Density Study of Pharmaceutical Nonlinear Optical Material: Melamine-Barbital Co-Crystal. <b>2015</b> , 119, 590-598	13

- 1965 Diversified self-association through OH $\cdots$ O hydrogen bonds in crystals of formylphenylboronic acid isomers. **2015**, 1083, 204-211 11
- 1964 Dicarboxylate recognition properties of a dinuclear copper(II) cryptate. **2015**, 54, 229-40 30
- 1963 Invariant and variable intermolecular interactions in functionalized malonic acid half-esters: X-ray, Hirshfeld surface and PIXEL energy analyses. **2015**, 17, 904-915 23
- 1962 A comparative study of the coordination behavior of -P and -As ligand complexes towards the trinuclear Lewis acid complex (perfluoro--phenylene)mercury. **2015**, 6, 132-139 37
- 1961 Synthesis and crystal structure of copper (II) uracil ternary polymeric complex with 1,10-phenanthroline along with the Hirshfeld surface analysis of the metal binding sites for the uracil ligand. **2015**, 1081, 14-21 8
- 1960 Methoxy- and methyl-substituted indole-3-acetonitrile (IAN): crystal structure and Hirshfeld surfaces analysis. **2015**, 41, 2915-2927
- 1959 Decomposition of Intermolecular Interactions in the Crystal Structure of Some Diacetyl Platinum(II) Complexes: Combined Hirshfeld, AIM, and NBO Analyses. **2016**, 21, 10
- 1958 Antibacterial Activity and Cytotoxicity of Silver(I) Complexes of Pyridine and (Benz)Imidazole Derivatives. X-ray Crystal Structure of [Ag(2,6-di(CH<sub>2</sub>OH)py)<sub>2</sub>]NO<sub>3</sub>. **2016**, 21, 87 41
- 1957 A non-solvated form of [(O--methyl--(2-methyl-phen-yl)-thio-carbamato- $\kappa$ -(tri-phenyl-phosphane- $\kappa$ )-gold(I): crystal structure and Hirshfeld surface analysis. **2016**, 72, 1446-1452 3
- 1956 Supramolecular solid-state architectures formed by co-crystallization of melamine and 2-, 3- and 4-chlorophenylacetic acids. **2016**, 1125, 493-502 9
- 1955 3-(benzo[d]thiazol-2-yl)phenol and 4-(benzo[d]thiazol-2-yl)phenol: Crystal Structure Determination, DFT Calculations and Visualizing Intermolecular Interactions Using Hirshfeld Surface Analysis. **2016**, 629, 120-134 5
- 1954 A method for fast safety screening of explosives in terms of crystal packing and molecular stability. **2016**, 22, 170 5
- 1953 Multi-functional supramolecular building blocks with hydroxy piperidino groups: new opportunities for developing nonlinear optical ionic crystals. **2016**, 18, 5832-5841 12
- 1952 Synergism in host-guest selectivity of picolinium chlorides by triphenylsilanol and triphenylmethanol. **2016**, 18, 5952-5958 3
- 1951 Intramolecular H $\cdots$ S interactions in metal di-(isopropyl)dithiocarbamate complexes. **2016**, 18, 7070-7077 9
- 1950 12-(3,4,5-Tri-meth-oxy-phen-yl)-2,3,4,12-tetra-hydro-1H-5-oxa-tetra-phen-1-one: crystal structure and Hirshfeld surface analysis. **2016**, 72, 809-14
- 1949 Effect of pressure on crystal structure and charge transport properties of 2,6-diphenylanthracene. **2016**, 31, 3731-3744 1
- 1948 Comparison of hydrogen bonds and diverse weak interactions of the nitro group in 2-methyl-4-nitroanilinium nitrate, bisulfate and two hexafluoridosilicates: elementary graph-set approach. **2016**, 72, 916-926 4

- 1947 Crystallographic and computational study of t-butyl N-[3-hydroxy-1-phenyl-4-(pyridin-2-ylsulfanyl)butan-2-yl]carbamate and its pyrimidin-2-yl analogue. **2016**, 231, 663-672
- 1946 A double stranded metal-organic assembly accommodating a pair of water trimers in the host cavity and catalysing Glaser coupling. **2016**, 72, 102-8 2
- 1945 Identification of Leishmania donovani Topoisomerase 1 inhibitors via intuitive scaffold hopping and bioisosteric modification of known Top 1 inhibitors. **2016**, 6, 26603 11
- 1944 A conformational polymorph of Ph<sub>3</sub>PAu[SC(OEt)=NPh] featuring an intramolecular Au<sup>III</sup> interaction. **2016**, 231, 653-661 11
- 1943 Anion-dependent structural diversity of cadmium(II) complexes: synthesis, crystal structures, luminescence properties, and unusual C-H/π supramolecular interactions involving aromatic M<sub>2</sub>X<sub>2</sub> cores. **2016**, 69, 1188-1205 6
- 1942 Single crystal X-ray diffraction and Hirshfeld surface analyses of supramolecular assemblies in certain hydrogen bonded heterocyclic organic crystals. **2016**, 1122, 146-156 27
- 1941 Photochromic Performance of Two Cu(II)-One-Dimensional Solvatomorphs Controlled by Intermolecular Interactions. **2016**, 16, 4026-4033 11
- 1940 Axial Mn-CCN Bonds of Cyano Manganese(II) Porphyrin Complexes: Flexible and Weak?. **2016**, 55, 5871-9 9
- 1939 Dimeric complexes of transition metal based on azole nucleating ligands involving hydrogen bonding interactions. **2016**, 115, 288-296 12
- 1938 Insights into the supramolecular features in isopropylmalonic and n-butylmalonic acids: Inputs from PIXEL and Hirshfeld surface analysis. **2016**, 1122, 29-36 9
- 1937 Supramolecular organic frameworks (SOFs) of tetrakis(4-hydroxyphenyl)porphyrin with efficient guest inclusion. **2016**, 18, 3372-3382 11
- 1936 A new tetranuclear copper(I) cluster of 1,3-bis(4-bromophenyl)triazene ligand: Synthesis, characterization, structural and computational studies. **2016**, 446, 32-40 2
- 1935 Counter-ion control of structure in uranyl ion complexes with 2,5-thiophenedicarboxylate. **2016**, 18, 1550-1562 26
- 1934 Two New Coordination Compounds Based on Polymeric, [CdCl<sub>3</sub>O] nB Chains or [Cd<sub>2.5</sub>Cl<sub>7</sub>O<sub>2</sub>] 2nB Layers: Synthesis, Crystal Structures, Physico-Chemical Properties and Theoretical Calculations. **2016**, 27, 1395-1417 9
- 1933 Quantitative Investigation of Polymorphism in 3-(Trifluoromethyl)-N-[2-(trifluoromethyl)phenyl]benzamide. **2016**, 16, 2561-2572 10
- 1932 Anchoring flexible uranyl dicarboxylate chains through stacking interactions of ancillary ligands on chiral U(VI) centres. **2016**, 18, 3905-3918 33
- 1931 Synthesis, single crystal structure, Hirshfeld surface and theoretical investigations on pyrimidine derivative. **2016**, 655-656, 17-29 13
- 1930 Structural analysis and physico-chemical characterization of mononuclear manganese(II) and polynuclear copper(II) complexes with pyridine-based alcohol. **2016**, 1126, 37-46 4

- 1929 Exploration of unconventional  $\pi$ -hole and  $\text{C-H}\cdots\text{H-C}$  types of supramolecular interactions in a trinuclear Cd(II) and a heteronuclear Cd(II)/Ni(II) complex and experimental evidence for preferential site selection of the ligand by 3d and 4d metal ions. **2016**, 6, 39376-39386 12
- 1928 Exploration of Intermolecular Interaction of One Silver(I) Polymer with Bis(pyrazolyl)methane Derivative: Experimental Observations, Hirshfeld Surface Analyses and Fluorescent Properties. **2016**, 26, 431-438 4
- 1927 Synthesis, crystal structure, Hirshfeld surface analysis and DNA binding properties of interactions with lattice pyrazinamide and its zinc(II) coordination polymer. **2016**, 42, 6947-6957 3
- 1926 Preliminary studies on unusual polymorphs of thymine: Structural comparison with other nucleobases. **2016**, 1120, 86-99 7
- 1925 Achirality in the low temperature structure and lattice modes of tris(acetylacetonate)iron(III). **2016**, 45, 8278-83 4
- 1924 Enantioselective synthesis of spirocyclic tetrahydrothiophene derivatives bearing a benzofuran-3(2H)-one scaffold. Unusual supramolecular crystal structure with high Z'. **2016**, 57, 2533-2538 14
- 1923 A family of complexes with N-scorpionate-type and other N-donor ligands obtained in situ from pyrazole derivative and zerovalent cobalt. Physicochemical and cytotoxicity studies. **2016**, 6, 44070-44079 8
- 1922 Growth, structural, dielectric, ferroelectric, and mechanical properties of l-prolinium tartrate single crystal. **2016**, 51, 7614-7623 11
- 1921 Supramolecular assembly of (Z)-ethyl 2-cyano-3-((4-fluorophenyl)amino) acrylate, crystal structure, Hirshfeld surface analysis and DFT studies. **2016**, 1120, 333-340 4
- 1920 Structural and Stability Studies of a Series of para-Phenylenediboronic and para-Hydroxyphenylboronic Acid Cocrystals with Selected Aromatic N-Oxides. **2016**, 16, 7037-7050 7
- 1919 Diverse supramolecular arrangement of substituted oxopyrrolidine analogues influenced by weak intermolecular interactions ( $\text{C-H}\cdots\text{O}/\text{C-H}\cdots\text{H}$ ). **2016**, 1122, 37-47 1
- 1918 Stereoselective Inhibitors Based on Nonpolar Hydrocarbons for Polar Organic Crystals. **2016**, 16, 6514-6521 2
- 1917 Synthesis and Characterization of 1:2 Complex of Mercury(II) Chloride with 1,3-Dimethyl-1H-Imidazole-2(3H)-Thione. **2016**, 86, 611-617 3
- 1916 Synthesis, crystal growth and characterization of di-valine maleic acid a new nonlinear optical material. **2016**, 6, 99139-99148 14
- 1915 Ring size effect on the solid state assembly of propargyl substituted hexa- and octacyclic peptoids. **2016**, 18, 8838-8848 12
- 1914 Isostructural polymorphs: qualitative insights from energy frameworks. **2016**, 18, 8497-8505 27
- 1913 Unique Axial Imidazole Geometries of Fully Halogenated Iron(II) Porphyrin Complexes: Crystal Structures and Mössbauer Spectroscopic Studies. **2016**, 55, 9632-9643 7
- 1912 A Sequential Method to Prepare Polymorphs and Solvatomorphs of  $[\text{Fe}(1,3\text{-bpp})_2](\text{ClO}_4)_2 \cdot n\text{H}_2\text{O}$  ( $n=0, 1, 2$ ) with Varying Spin-Crossover Behaviour. **2016**, 22, 12767-76 44

1911	Experimental and theoretical charge density assessments for the 4-perfluoropyridyl- and 4-perfluorophenyl-1,2,3,5-dithiadiazolyl radicals. <b>2016</b> , 18, 7116-7125	13
1910	Supramolecular Cd(II) complexes with (E)-N,N'-bis(2-pyridyl)iminoisoindoline (2-pyimiso): synthesis, X-ray structures, Hirshfeld surface analyses, and DFT study of [CdX <sub>2</sub> (2-pyimiso) <sub>2</sub> ] (X = Cl or NCS)** Present address: Nanobusiness Informa <sup>ç</sup> o e Inova <sup>ç</sup> o Ltda, Incubadora de Projetos, Instituto Nacional de Metrologia, Qualidade e Tecnologia, Duque de Caxias RJ, 25250-020, Brazil. View all papers <b>2016</b> , 60, 3361-3383	3
1909	Conformational adjustments over synthons of urea and thiourea based assemblies. <b>2016</b> , 18, 7753-7763	9
1908	Ruthenium Lewis Acid-Catalyzed Asymmetric Diels-Alder Reactions: Reverse-Face Selectivity for $\beta,\mu$ Unsaturated Aldehydes and Ketones. <b>2016</b> , 99, 774-789	4
1907	Synthesis, crystal structure and Hirshfeld surface analysis of copper(II) complexes: DNA- and BSA-binding, molecular modeling, cell imaging and cytotoxicity. <b>2016</b> , 119, 23-38	17
1906	Growth, morphology, structure and characterization of L-histidinium dihydrogen arsenate orthoarsenic acid single crystal. <b>2016</b> , 72, 593-601	6
1905	Magnetic Bistability in Macrocycle-Based FeII Spin-Crossover Complexes: Counter Ion and Solvent Effects. <b>2016</b> , 2016, 5305-5314	11
1904	Two di-alkyl-ammonium salts of 2-amino-4-nitro-benzoic acid: crystal structures and Hirshfeld surface analysis. <b>2016</b> , 72, 1691-1699	3
1903	A new end-on (1,1) azido bridged [Zn <sub>2</sub> (L) <sub>2</sub> (Na) <sub>3</sub> ] <sub>n</sub> 1D chain derived from a trinuclear zinc complex: syntheses, crystal structures, photoluminescence properties and DFT study. <b>2016</b> , 69, 3092-3106	8
1902	Homoleptic Phosphaalkyne Complexes of Silver(I). <b>2016</b> , 55, 13301-13305	6
1901	Solvatomorphism in (Z)-4-fluoro-N'-(3-fluorophenyl)benzimidamide: the role of intermolecular O-H...F interaction. <b>2016</b> , 18, 8291-8300	3
1900	Alkyl Spacer Length and Protonation Induced Changes in Crystalline Psychoactive Arylpiperazine Derivatives: Single-Crystal X-ray, Solid-State NMR, and Computational Studies. <b>2016</b> , 16, 6371-6380	5
1899	DFT(B3LYP/LanL2DZ), non-linear optical and electrical studies of a new hybrid compound: [C <sub>6</sub> H <sub>10</sub> (NH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub> [CoCl <sub>4</sub> ·2H <sub>2</sub> O]. <b>2016</b> , 84, 384-394	20
1898	Hydrogen Bonding versus Halogen Bonding in Host-Guest Compounds. <b>2016</b> , 16, 4765-4771	10
1897	Enhanced selectivity towards xylene isomers of a mixed ligand Ni(II) thiocyanato complex. <b>2016</b> , 119, 127-133	16
1896	Coordination-Induced Molecular Tweezing: Ruthenium Clusters Docked at Azuliporphyrinogens. <b>2016</b> , 55, 12061-12073	8
1895	Enhanced Intermolecular Hydrogen Bonds Facilitating the Highly Dense Packing of Energetic Hydroxylammonium Salts. <b>2016</b> , 16, 7231-7239	41
1894	Growth and structural and physical properties of diisopropylammonium bromide molecular single crystals. <b>2016</b> , 49, 2053-2062	36

- 1893 In Silico Quantum Chemical and Crystallographic Treatment of  $\beta$ -Formylketene Dithioacetal towards the Elucidation of Its Structural and Optical Nature. **2016**, 1, 5974-5981 7
- 1892 Pyridyl-phenylethynylene bis-urea macrocycles: self-assembly and utility as a nanoreactor for the selective photoreaction of isoprene. **2016**, 6, 98350-98355 7
- 1891 Exploration of structural motifs influencing solid-state conformation and packing of unclosed cryptands sharing the same 19-membered macrocyclic core. **2016**, 72, 8373-8381 8
- 1890 The role of unconventional stacking interactions in the supramolecular assemblies of Hg(II) coordination compounds. **2016**, 18, 9056-9066 34
- 1889 Energy frameworks and a topological analysis of the supramolecular features in in situ cryocrystallized liquids: tuning the weak interaction landscape via fluorination. **2016**, 18, 31811-31820 39
- 1888 Homoleptic Phosphaalkyne Complexes of Silver(I). **2016**, 128, 13495-13499 3
- 1887 Zwitterionic 4-bromo-6-methoxy-2-[[tris-(hydroxy-methyl)methyl]-iminiumyl-methyl]phenolate: crystal structure and Hirshfeld surface analysis. **2016**, 72, 1223-7 1
- 1886 A monoclinic polymorph of [(Z)-N-(3-chloro-phenyl)-O-methyl-thio-carbamato- $\beta$ ](tri-phenyl-phosphane- $\beta$ )gold(I): crystal structure and Hirshfeld surface analysis. **2016**, 72, 1068-73 1
- 1885 In Situ Tailor-Made Additives for Molecular Crystals: A Simple Route to Morphological Crystal Engineering. **2016**, 16, 3555-3561 12
- 1884 Physicochemical characterization and decomposition kinetics of (S)-4-[1-(2,3-dimethylphenyl)ethyl]-3H-imidazole HCl/S-enantiomer of medetomidineHCl. **2016**, 124, 269-278 1
- 1883 Two carbamate derivatives with Z=2 and 3: An interplay of strong and weak hydrogen bonds. **2016**, 1122, 290-298 4
- 1882 Solvent and anion facilitated conformational changes in benzylamine substituted thiazolamine. **2016**, 40, 6899-6906 2
- 1881 Synthesis, vibrational, electrostatic potential and NMR studies of (E and Z) 1-(4-chloro-3-nitrophenyl)-3-(2-methoxyphenyl)triazene: Combined experimental and DFT approaches. **2016**, 1125, 247-259 4
- 1880 Intermolecular interactions and chiral crystallization effects in (1,5,3-dithiazepan-3-yl)-alkanoic acids. **2016**, 18, 5686-5696 3
- 1879 Structural investigation of (2E)-2-(ethoxycarbonyl)-3-[(4-methoxyphenyl)amino]prop-2-enoic acid: X-ray crystal structure, spectroscopy and DFT. **2016**, 1119, 259-268 17
- 1878 Quantitative relationships between structure and cytotoxic activity of flavonoid derivatives. An application of Hirshfeld surface derived descriptors. **2016**, 26, 3336-3341 14
- 1877 (2Z)-3-Hydroxy-1-(pyridin-2-yl)-3-(pyridin-3-yl)prop-2-en-1-one: crystal structure and Hirshfeld surface analysis. **2016**, 72, 849-53 3
- 1876 Density functional theory calculations of the nitrogen-rich energetic compound 3,4-diamino-1,2,4-triazolium 1-aminotetrazol-5-oneate. **2016**, 121, 225-231



1875	Selective picomolar level fluorometric sensing of the Cr(VI)-oxoanion in a water medium by a novel metal-organic complex. <b>2016</b> , 6, 61966-61973		9
1874	Molecular structure, experimental and theoretical spectroscopic characterization and non-linear optical properties studies of a new non-centrosymmetric hybrid material. <b>2016</b> , 1123, 144-152		19
1873	Anion directed structural diversity in zinc complexes with conformationally flexible quinazoline ligand: structural, spectral and theoretical studies. <b>2016</b> , 45, 12053-68		7
1872	Crystal structure and Hirshfeld-surface analysis of (benzene-carbo-thio-amide- $\kappa$ )bromido-bis-(tri-phenylphosphane- $\kappa$ )silver(I). <b>2016</b> , 72, 984-7		1
1871	Experimental and theoretical charge-density analysis of 1,4-bis(5-hexyl-2-thienyl)butane-1,4-dione: applications of a virtual-atom model. <b>2016</b> , 72, 75-86		2
1870	A library of dimeric and trimeric phthalonitriles linked by a single aromatic ring: comparative structural and DFT investigations. <b>2016</b> , 18, 1416-1426		11
1869	'Quasi-isostructural polymorphism' in molecular crystals: inputs from interaction hierarchy and energy frameworks. <i>Chemical Communications</i> , <b>2016</b> , 52, 2141-4	5.8	35
1868	A Triazolate-Supported Fe <sub>3</sub> ( $\mu$ -O) Core: Crystal Structure, Fluorescence, and Hirshfeld Surface Analysis. <b>2016</b> , 27, 1181-1190		7
1867	Crystal Structures and Hirshfeld Surface Analyses of 6-Substituted Chromones. <b>2016</b> , 46, 170-180		8
1866	A New Solvothermal Synthetic Route Yields the New Thio- $\kappa$ stannate [La(dien) <sub>3</sub> ] <sub>2</sub> [Sn <sub>2</sub> S <sub>6</sub> ]Cl <sub>2</sub> . <b>2016</b> , 642, 25-30		3
1865	Synthesis, crystal structure and cytotoxic activity of ruthenium(II) piano-stool complex with N,N-chelating ligand. <b>2016</b> , 1126, 74-82		13
1864	Why Do Chemically Similar Pharmaceutical Molecules Crystallize in Different Structures: A Case of Droperidol and Benperidol. <b>2016</b> , 16, 1643-1653		10
1863	Supramolecular self-assembly of a coumarine-based acylthiourea synthon directed by $\pi$ -stacking interactions: Crystal structure and Hirshfeld surface analysis. <b>2016</b> , 1111, 76-83		42
1862	Two new palladium and platinum complexes with a bidentate pyrazole-based ligand: crystal structure, fluorescence and Hirshfeld surface analysis. <b>2016</b> , 13, 823-830		4
1861	Salts of phenylacetic acid and 4-hydroxyphenylacetic acid with Cinchona alkaloids: Crystal structures, thermal analysis and FTIR spectroscopy. <b>2016</b> , 1114, 30-37		4
1860	Growth, crystal structure, Hirshfeld surface, dielectric and mechanical properties of a new organic single crystal: Bis glycine- $\kappa$ squarate. <b>2016</b> , 6, 24565-24576		23
1859	A Capped Dipeptide Which Simultaneously Exhibits Gelation and Crystallization Behavior. <b>2016</b> , 32, 2245-50		27
1858	Quantifying intermolecular interactions in solid state indapamide and other popular diuretic drugs: Insights from Hirshfeld surface study. <b>2016</b> , 1116, 22-29		11

1857	Polymorphs and Versatile Solvates of 7-Hydroxyisoflavone. <b>2016</b> , 105, 1387-97	12
1856	Porphyrin-based assemblies directed by non-covalent interactions: highlights of recent investigations. <b>2016</b> , 18, 3318-3339	28
1855	Correlating the melting point alteration with the supramolecular structure in aripiprazole drug cocrystals. <b>2016</b> , 18, 1024-1038	15
1854	Salts of Tryptophan with p-Toluenesulphonic Acid and Camphorsulphonic Acids. <b>2016</b> , 46, 57-66	1
1853	Tetranuclear manganese(II) complexes of hydrazone and carbohydrazone ligands: Synthesis, crystal structures, magnetic properties, Hirshfeld surface analysis and DFT calculations. <b>2016</b> , 443, 101-109	24
1852	Synthesis, X-ray characterization, DFT calculations and Hirshfeld surface analysis studies of carbohydrazone based on Zn(II) complexes. <b>2016</b> , 18, 102-112	28
1851	Crystallization induced enhanced emission in conformational polymorphs of a rotationally flexible molecule. <b>2016</b> , 4, 2931-2935	17
1850	Crystal structures and Hirshfeld surface analysis calculations of mercury(II) complexes with a diiminopyridine ligand. <b>2016</b> , 1105, 159-168	5
1849	Framework deformation of the microporous vanadium benzenedicarboxylate MIL-47 upon absorption of organosulfur molecules. <b>2016</b> , 219, 112-116	6
1848	Crystal structure, Hirshfeld surfaces and DFT computation of NLO active (2E)-2-(ethoxycarbonyl)-3-[(1-methoxy-1-oxo-3-phenylpropan-2-yl)amino] prop-2-enoic acid. <b>2016</b> , 153, 625-36	149
1847	Intermolecular interactions in polymorphs of the cyclic trimeric perfluoro-ortho-phenylene mercury from geometric, energetic and AIM viewpoints: DFT study and Hirshfeld surface analysis. <b>2016</b> , 27, 37-49	8
1846	Nickel(II) complex of 4-amino-N-(2-pyrimidinyl)benzenesulfonamide: Synthesis, spectroscopic characterization, antimicrobial activity, crystal structure, and Hirshfeld surface analysis. <b>2017</b> , 47, 234-243	2
1845	How do halogen bonds (S-O?I, N-O?I and C-O?I) and halogen-halogen contacts (C-I?I-C, C-F?F-C) subsist in crystal structures? A quantum chemical insight. <b>2017</b> , 23, 16	7
1844	Molecular and supramolecular properties of a Hg(II) complex with (E)-N,N'-bis(2-pyridyl)iminoindoline: synthesis, spectroscopy, X-ray structure and Hirshfeld surface analyses, and DFT calculations. <b>2017</b> , 70, 1089-1104	4
1843	Synthesis, characterization, and computational study of the supramolecular arrangement of a novel cinnamic acid derivative. <b>2017</b> , 23, 35	7
1842	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. <b>2017</b> , 1134, 492-503	20
1841	Supramolecular association in (2-pyrazine)-tetrakis(N,N-bis(2-hydroxyethyl)dithiocarbamate)dizinc(II) and its di-dioxane solvate. <b>2017</b> , 232, 287-298	14
1840	Modelling, structural, thermal, optical and vibrational studies of a new organic/inorganic hybrid material (C <sub>5</sub> H <sub>16</sub> N <sub>2</sub> )Cd <sub>1.5</sub> Cl <sub>5</sub> . <b>2017</b> , 40, 55-66	7

- 1839 Chiral Crystals of an Achiral Molecule Exhibit Plastic Bending and a Crystal-to-Crystal Phase Transition. **2017**, 17, 1390-1395 13
- 1838 Hydrothermal synthesis, structural elucidation, spectroscopic studies, thermal behavior and luminescence properties of a new 3-d'compound: FeAlF<sub>2</sub>(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)(HPO<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O). **2017**, 1134, 797-805 7
- 1837 Approaching an experimental electron density model of the biologically active trans-epoxysuccinyl amide groupSubstituent effects vs. crystal packing. **2017**, 30, e3683 4
- 1836 Synthesis, growth, structural characterization, Hirshfeld analysis and nonlinear optical studies of a methyl substituted chalcone. **2017**, 1136, 244-252 47
- 1835 New Electro-Optic Salt Crystals for Efficient Terahertz Wave Generation by Direct Pumping at Ti:Sapphire Wavelength. **2017**, 5, 1600758 16
- 1834 The first coordination compounds of OP[NC<sub>4</sub>H<sub>8</sub>O]<sub>3</sub> phosphoric triamide ligand: structural study and Hirshfeld surface analysis of SnIV and MnII complexes. **2017**, 70, 1285-1302 4
- 1833 Simultaneous enhancements of solubility and dissolution rate of poorly water-soluble febuxostat via salts. **2017**, 1137, 328-334 8
- 1832 Rage Against Conformity: Ruthenium(II) Bisterpyridine Complexes Respond to Crystal Engineering Instructions with Whelming Results. **2017**, 70, 529 2
- 1831 Synthesis and crystal structures of three new lead(II) isonicotinoylhydrazone derivatives: Anion controlled nuclearity and dimensionality. **2017**, 461, 192-205 26
- 1830 Phenylacetic acid co-crystals with acridine, caffeine, isonicotinamide and nicotinamide: Crystal structures, thermal analysis, FTIR spectroscopy and Hirshfeld surface analysis. **2017**, 1139, 60-66 8
- 1829 Supramolecular Chemistry of BrettPhos and BrettPhos Oxide: Breakup of Isostructurality via OrderDisorder Phase Transitions. **2017**, 17, 1982-1990 6
- 1828 Dicyano- and tetracyanopentacene: foundation of an intriguing new class of easy-to-synthesize organic semiconductors. **2017**, 5, 2603-2610 12
- 1827 Hydrogen bonded R22(8) graph set in inducing charge transfer mechanism in guanidinium-3,5-dinitrobenzoate: A combined experimental, theoretical and Hirshfeld surface study. **2017**, 1137, 649-662 36
- 1826 Structure directing role of amines and water molecules in the self-assembly of polyoxomolybdates. **2017**, 19, 2021-2035 4
- 1825 -Aceto-nitrile-tricarbon-yl(di-methyl-carbamodi-thio-ato- $\eta$ )rhenium(I): crystal structure and Hirshfeld surface analysis. **2017**, 73, 213-218 2
- 1824 Three oxime ether derivatives: Synthesis, crystallographic study, electronic structure and molecular electrostatic potential calculation. **2017**, 1137, 615-625 5
- 1823 AgI and PbII as Additional Assembling Cations in Uranyl Coordination Polymers and Frameworks. **2017**, 17, 2116-2130 32
- 1822 Supramolecular assembly in the epiisopiloturine hydrochloride salt. **2017**, 1136, 204-213 1

1821	Weak Interactions Cause Packing Polymorphism in Pharmaceutical Two-Component Crystals. The Case Study of the Salicylamide Cocrystal. <b>2017</b> , 17, 1425-1437	26
1820	Structural analyses of two new highly distorted octahedral copper(II) complexes with quinoline-type ligands; Hirshfeld, AIM and NBO studies. <b>2017</b> , 127, 36-50	15
1819	Terahertz Phonon Mode Engineering of Highly Efficient Organic Terahertz Generators. <b>2017</b> , 27, 1605583	31
1818	Synthesis, characterization, and in vitro evaluation and in silico molecular docking of thiourea derivatives incorporating 4-(trifluoromethyl)phenyl moiety. <b>2017</b> , 1139, 149-159	25
1817	The first C(O)NHP(O)-based phosphoric triamide structure with an N-H...O hydrogen bonding: A combination of X-ray crystallography and theoretical study to evaluate the strength of hydrogen bonds. <b>2017</b> , 192, 936-944	3
1816	Close insight into the nature of intermolecular interactions in dihydropyrimidine-2(1H)-thione derivatives. <b>2017</b> , 19, 1495-1508	19
1815	Different molecular assemblies in two new phosphoric triamides with the same C(O)NHP(O)(NH) <sub>2</sub> skeleton: crystallographic study and Hirshfeld surface analysis. <b>2017</b> , 71, 1809-1823	3
1814	Synthesis, characterization, Hirshfeld surfaces and DFT computation of novel benzyl N-(1,3-benzothiazol-2-yl)-N-benzylcarbamate. <b>2017</b> , 1143, 135-145	
1813	The 1:1 co-crystal of 2-bromo-naphthalene-1,4-dione and 1,8-di-hydroxy-anthracene-9,10-dione: crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 738-745	4
1812	Geometry dependence of electron donating or accepting abilities of amine groups in 4,4'-disulfanediybis(methylene)dithiazol-2-amine: Pyramidal versus planar. <b>2017</b> , 1141, 650-659	2
1811	Ionic Couple-Driven Palladium Leaching by Organic Triiodide Solutions. <b>2017</b> , 5, 4359-4370	8
1810	A novel multi-nitrogen 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane-based energetic co-crystal with 1-methyl-3,4,5-trinitropyrazole as a donor: experimental and theoretical investigations of intermolecular interactions. <b>2017</b> , 41, 4165-4172	41
1809	Role of halogen atoms in the formation of one-dimensional Cu(I) coordination polymers based on 2-amino-5-halopyrimidine. <b>2017</b> , 1144, 173-180	1
1808	Crystal structure, Hirshfeld surface analysis, vibrational, thermal behavior and UV spectroscopy of (2,6-diaminopyridinium) dihydrogen arsenate. <b>2017</b> , 1145, 121-131	20
1807	Growth, crystal structure, Hirshfeld surface, optical, piezoelectric, dielectric and mechanical properties of bis(L-asparaginium hydrogensquarate) single crystal. <b>2017</b> , 73, 347-359	22
1806	Enhancing intermolecular interactions and their anisotropy to build low-impact-sensitivity energetic crystals. <b>2017</b> , 19, 3145-3155	27
1805	Molecular and crystalline architectures based on HgI <sub>2</sub> : from metallamacrocycles to coordination polymers. <b>2017</b> , 19, 3322-3330	6
1804	A 2D Co(II) Coordination Polymer Containing Tri-flexural Helical Chains from Achiral Materials. <b>2017</b> , 27, 1190-1198	1

1803	Synthesis, molecular and solid state structure of 5-(5-nitro furan-2-ylmethylene), 3- N -(2-methoxy phenyl), 2- N ?-(2-methoxyphenyl) imino thiazolidin-4-one: X-ray powder diffraction and DFT studies. <b>2017</b> , 1143, 259-264	6
1802	The non-coordinating anion 1,1,3,3-tetracyano-2-propoxy-propenide as an anion- $\pi$ donor in cis-diaquabis(2,2'-dipyridylamine)zinc and its cadmium analog: Luminescence properties, Hirshfeld analysis and central-atom induced polymorphism. <b>2017</b> , 131, 27-33	7
1801	Hydrazinium 2-amino-4-nitro-benzoate dihydrate: crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 579-585	3
1800	Salts and Cocrystals of Furosemide with Pyridines: Differences in $\pi$ -Stacking and Color Polymorphism. <b>2017</b> , 17, 3071-3087	16
1799	Designing a new cocrystal of olanzapine drug and observation of concomitant polymorphism in a ternary cocrystal system. <b>2017</b> , 19, 355-366	13
1798	Occurrence of 3D isostructurality in fluorinated phenyl benzamidines. <b>2017</b> , 19, 47-63	11
1797	Crystal Engineering of 6-Carboxy-4-aryl-2,2'-bipyridine Complexes: Potent Chelators with Intrinsic Intermolecular Affinity. <b>2017</b> , 17, 4365-4376	5
1796	Hydrogen Bond-Directed Cruciform and Stacked Packing of a Pyrrole-Based Azaphenacene. <b>2017</b> , 17, 3371-3378	9
1795	Theoretical investigations into the charge transfer properties of thiophene $\pi$ -substituted naphthodithiophene diimides: excellent n-channel and ambipolar organic semiconductors. <b>2017</b> , 19, 13978-13993	25
1794	Synthesis, characterization and theoretical study in gaseous and solid phases of the imine 4-Acetyl-N-(4-methoxybenzylidene)aniline. <b>2017</b> , 1147, 300-309	1
1793	Structural, vibrational and optical properties of a new self assembled organic/inorganic crystal (C <sub>4</sub> H <sub>7</sub> N <sub>2</sub> ) [CdCl <sub>3</sub> (H <sub>2</sub> O)]. <b>2017</b> , 28, 12698-12710	7
1792	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. <b>2017</b> , 105, 226-237	9
1791	Complex electronic interplay of $\pi$ -hole and $\sigma$ -hole interactions in crystals of halogen substituted 1,3,4-oxadiazol-2(3H)-thiones. <b>2017</b> , 19, 3485-3498	13
1790	The effect of chalcogen substitution on the structure and spectroscopy of 4,7-dimethyl-2H-chromen-2-one/thione analogues. <b>2017</b> , 41, 5770-5783	3
1789	Theoretical investigations of nonlinear optical properties of two crystalline acetamides structures including polarization effects of their environment. <b>2017</b> , 681, 110-123	18
1788	Synthesis, structural and biological studies of two new Co(III) complexes with tridentate hydrazone ligand derived from the antihypertensive drug hydralazine. <b>2017</b> , 466, 16-29	17
1787	Solid-state structure of 1-(diaminomethylene)thiourea-1-ium propionate. <b>2017</b> , 1145, 222-229	6
1786	Probing the Effects of Ligand Field and Coordination Geometry on Magnetic Anisotropy of Pentacoordinate Cobalt(II) Single-Ion Magnets. <b>2017</b> , 56, 6870-6878	49

1785	Predicting the Position of the Hydrogen Atom in the Short Intramolecular Hydrogen Bond of the Hydrogen Maleate Anion from Geometric Correlations. <b>2017</b> , 17, 3812-3825	16
1784	Syntheses, X-ray Crystal Structures, Photoluminescence Properties, Antimicrobial Activities and Hirshfeld Surface of Two New Cd(II) Azide/Thiocyanate Linked Coordination Polymers. <b>2017</b> , 2, 4811-4822	17
1783	Synthesis, single crystal X-ray, Hirshfeld surface analysis and characterization of novel 4-(2,4-dichlorophenyl)-N-(2,6-dichlorophenyl)-1,3-thiazol-2-amine. <b>2017</b> , 1146, 490-498	3
1782	Hydrogen bonding interactions and supramolecular assemblies in 2-amino guanidinium 4-methyl benzene sulphonate crystal structure: Hirshfeld surfaces and computational calculations. <b>2017</b> , 1146, 723-734	28
1781	A potential Cu/V-organophosphonate platform for tailored void spaces via terpyridine mold casting. <b>2017</b> , 73, 296-303	13
1780	Directional O...F halogen bonds. <b>2017</b> , 73, 136-137	10
1779	Synthesis, structural characterization and quantum chemical calculations on 1-(isomeric methylbenzoyl)-3-(4-trifluoromethylphenyl)thioureas. <b>2017</b> , 1141, 309-321	23
1778	Diiodomethane as a halogen bond donor toward metal-bound halides. <b>2017</b> , 19, 2517-2525	56
1777	Synthesis, crystal structure, vibrational spectroscopy and photoluminescence of new hybrid compound containing chlorate anions of stanate (II). <b>2017</b> , 1141, 660-667	17
1776	Structural characterization and physicochemical features of new hybrid compound containing chlorate anions of cadmate (II). <b>2017</b> , 1141, 390-399	12
1775	Trityl Group as an Crystal Engineering Tool for Construction of Inclusion Compounds and for Suppression of Amide NH...O?C Hydrogen Bonds. <b>2017</b> , 17, 2560-2568	12
1774	Reversible crystal-to-crystal chiral resolution: making/breaking non-bonding SO interactions. <i>Chemical Communications</i> , <b>2017</b> , 53, 3964-3966	5.8 6
1773	Characterization of fluorine-centred 'F...O' Hole interactions in the solid state. <b>2017</b> , 73, 140-152	23
1772	New cadmium(II) and zinc(II) coordination polymers derived from a pyridine-hydrazone block: Self-assembly generation, structural and topological features, and theoretical analysis. <b>2017</b> , 458, 68-76	11
1771	Structural study, intermolecular interactions in view of X-ray and Hirshfeld surface analysis, DSC characterization, and electrical properties of bis-(4-benzylpyridinium) tetrabromozincate. <b>2017</b> , 23, 1173-1186	4
1770	Understanding the conformational changes and molecular structure of furoyl thioureas upon substitution. <b>2017</b> , 176, 8-17	25
1769	Unusual physical behaviour and polymorphic phase transitions in crystalline bicyclic anhydrides. <b>2017</b> , 19, 276-284	2
1768	Coordination Polymers with Intramolecular Fluorine-Involved Contacts in Two-Dimensional Sheet Windows. <b>2017</b> , 17, 834-845	18

- 1767 Iso-Structurality Induced Solid Phase Transformations: A Case Study with Lenalidomide. **2017**, 17, 612-628 18
- 1766 Synthesis, crystal structure and theoretical analysis of intermolecular interactions in two biologically active derivatives of 1,2,4-triazoles. **2017**, 1134, 426-434 10
- 1765 New Charge-Transfer Complexes with 1,2,5-Thiadiazoles as Both Electron Acceptors and Donors Featuring an Unprecedented Addition Reaction. **2017**, 23, 852-864 19
- 1764 Electrophilic-Nucleophilic Dualism of Nickel(II) toward Ni<sup>4+</sup> Noncovalent Interactions: Semicoordination of Iodine Centers via Electron Belt and Halogen Bonding via  $\pi$ -Hole. **2017**, 56, 13562-13578 66
- 1763 Designing Solid Solutions of Enantiomers: Lack of Enantioselectivity of Chiral Naphthalimide Derivatives in the Solid State. **2017**, 17, 6477-6485 12
- 1762 An insight into the synthesis, crystal structure, geometrical modelling of crystal morphology, Hirshfeld surface analysis and characterization of N-(4-methylbenzyl)benzamide single crystals. **2017**, 50, 1498-1511 20
- 1761 Solid-State Characterization and Insight into Transformations and Stability of Apatinib Mesylate Solvates. **2017**, 17, 5994-6005 18
- 1760 Iron(II) Bis(imidazole) Derivatives of a Binuclear Porphyrin Model: Crystal Structures and Mössbauer Properties. **2017**, 56, 12615-12624 4
- 1759 Halogen bonding, chalcogen bonding, pnictogen bonding, tetrel bonding: origins, current status and discussion. **2017**, 203, 485-507 115
- 1758 On the Formation and Desolvation Mechanism of Organic Molecule Solvates: A Structural Study of Methyl Cholate Solvates. **2017**, 17, 5712-5724 22
- 1757 A Combined Theoretical Calculation and Hirshfeld Surface Analysis of Cooperative Non-covalent Interactions in the Crystal Packing in [Cu(L1)2(EDA)]. **2017**, 643, 1245-1252 9
- 1756 Diversity of Isomerization Patterns and Protolytic Forms in Aminocarbene PdII and PtII Complexes Formed upon Addition of N,N'-Diphenylguanidine to Metal-Activated Isocyanides. **2017**, 36, 4145-4159 16
- 1755 Experimental and theoretical spectroscopic and structural analyses of a new chalcone single crystal derived from 4-bromo-2-thiophenecarboxaldehyde. **2017**, 650, 87-101 4
- 1754 A New Organic/Inorganic Hybrid Compound (C<sub>7</sub>H<sub>7</sub>N<sub>2</sub>)<sub>2</sub>[Cu<sub>2</sub>Cl<sub>6</sub>]: Synthesis, Crystal Structure, Hirshfeld Surface Analysis, Vibrational and Thermal Properties. **2017**, 28, 3021-3034 2
- 1753 Evaluation of the Role of Isostructurality in Fluorinated Phenyl Benzoates. **2017**, 17, 5117-5128 11
- 1752 The Hirshfeld surface of three new isonicotinylhydrazine co-crystals: Comparison of hydrogen bonds and crystal structures. **2017**, 1150, 586-594 2
- 1751 Benzyl Dihydrazone versus Thiosemicarbazone Schiff Base: Effects on the Supramolecular Arrangement of Cobalt Thiocyanate Complexes and the Generation of CoN<sub>6</sub> and CoN<sub>4</sub>S<sub>2</sub> Coordination Spheres. **2017**, 2017, 4763-4772 37
- 1750 Efficient and thermally stable inverted perovskite solar cells by introduction of non-fullerene electron transporting materials. **2017**, 5, 20615-20622 62

1749	Tautomerism in acyl-pyrazolones and in a novel photolysis product Importance and impact of the accurate localization of hydrogen atoms in crystal structures. <b>2017</b> , 28, 1343-1357	4
1748	Synthesis, spectroscopic characterization, fluorescence properties of new silver(I) complexes with optically active Schiff bases and their application in thin layers deposition. <b>2017</b> , 135, 153-160	6
1747	Structural organization in the trimethylamine iodine monochloride complex. <b>2017</b> , 19, 5194-5201	3
1746	Transesterification reactions of dimethoxycarbonyl ethyltin- morpholinodithiocarbamate, [(MeO <sub>2</sub> CCH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> Sn(MDTC) <sub>2</sub> ]: Synthesis, spectroscopy, X-ray structural characterization and DFT calculations of new diestertin dithiocarbamate complexes [Part II. <b>2017</b> , 135, 161-168	1
1745	Exploring potent ligand for proteins: insights from knowledge-based scoring functions and molecular interaction energies. <b>2017</b> , 28, 1537-1552	3
1744	A Chiral Metal-Organic Material that Enables Enantiomeric Identification and Purification. <b>2017</b> , 3, 281-289	65
1743	Crystal structure studies, Hirshfeld surface analysis and DFT calculations of novel 1-[5-(4-methoxy-phenyl)-[1,3,4]oxadiazol-2-yl]-piperazine derivatives. <b>2017</b> , 11-12, 40-58	7
1742	Water-Encapsulated Ni(II) Salphen-Type Host Complexes: Experimental and Theoretical Analysis of Potentially Bioactive Quasi-Isostructural Polymorphs. <b>2017</b> , 2, 6493-6502	7
1741	Crystal growth, structural, optical, thermal and dielectric properties of lithium hydrogen oxalate monohydrate single crystal. <b>2017</b> , 73, 154-162	18
1740	Photochemical and Electrochemical Triggered Bis(hydrazone) Switch. <b>2017</b> , 23, 14872-14882	19
1739	Solvent-Mediated Reversible Structural Transformation of Mercury Iodide Coordination Polymers: Role of Halide Anions. <b>2017</b> , 17, 4801-4809	23
1738	Quantitative investigation of C-H...O and other intermolecular interactions in a series of crystalline N-(substituted phenyl)-2-naphthamide derivatives. <b>2017</b> , 19, 5473-5491	10
1737	Does increasing pressure always accelerate the condensed material decay initiated through bimolecular reactions? A case of the thermal decomposition of TKX-50 at high pressures. <b>2017</b> , 19, 23309-23317	6
1736	Bis-Imine Boronic Esters Obtained by One-Step Multicomponent Reactions. Synthesis and X-Ray Diffraction Structural Analysis. <b>2017</b> , 2, 11265-11272	0
1735	New pharmaceutical salts containing pyridoxine. <b>2017</b> , 73, 1064-1070	4
1734	An exploration into the amide...pseudo amide hydrogen bonding synthon between a new coformer with two primary amide groups and theophylline. <b>2017</b> , 19, 7112-7124	6
1733	Studying the fluorescence conversion in organic charge transfer cocrystals of chalcone derivatives and TCNB. <b>2017</b> , 41, 14610-14617	2
1732	Structural and computational study of 1,2,4-triazolin-5-thione derivative and its DMSO solvate. <b>2017</b> , 1147, 786-796	1



1731	Synthesis, structural characterization and cytotoxic activity against tumor cells of heteroleptic copper (I) complexes with aromatic diimines and phosphines. <b>2017</b> , 466, 559-564	12
1730	Structural elucidation, theoretical investigation using DFT calculations, thermal and dielectric analyses of new zinc(II) based inorganic-organic hybrid. <b>2017</b> , 28, 642-650	6
1729	Molecular modelling of an organic salt 4-chloroanilinium hydrogen malonate (4CAHM): crystal structure, theoretical and Hirshfeld surface analysis. <b>2017</b> , 21, 304-312	2
1728	Solvent dependent nuclearity of manganese complexes with a polydentate hydrazone-based ligand and thiocyanate anions. <b>2017</b> , 455, 204-212	6
1727	Octahedral Ni(II) complex with new NNO donor Schiff base ligand: Synthesis, structure and Hirshfeld surface. <b>2017</b> , 1130, 844-854	9
1726	Quantitative analysis of weak interactions by Lattice energy calculation, Hirshfeld surface and DFT studies of sulfamonomethoxine. <b>2017</b> , 1128, 127-134	13
1725	Elaboration, structural, spectroscopy, DSC investigations and Hirshfeld surface analysis of a one-dimensional self-assembled organic-inorganic hybrid compound. <b>2017</b> , 1128, 205-214	10
1724	Vibrational spectroscopic (FT-IR, FT-Raman) studies, Hirshfeld surfaces analysis, and quantum chemical calculations of m-acetotoluidide and m-thioacetotoluidide. <b>2017</b> , 1128, 619-628	7
1723	Synthesis, structural characterization, Hirshfeld surface analysis, spectroscopic and ferroelectric properties studies of 4-methylbenzylammonium sulfate. <b>2017</b> , 90, 557-568	2
1722	On the molecular and supramolecular properties of N,N'-disubstituted iminoisoindolines: Synthesis, spectroscopy, X-ray structure and Hirshfeld surface analyses, and DFT calculations of two (E)-N,N'-bis(aryl)iminoisoindolines (aryl = 2-tert-butylphenyl or perfluorophenyl). <b>2017</b> , 1130, 165-173	30
1721	Synthesis, crystal growth, structural evaluation and nonlinear optical analysis of ethyl-4-(3,4-dimethoxyphenyl)-6-methyl-2-sulfanylidene-3,4-dihydro-1H-pyrimidine-5-carboxylate. <b>2017</b> , 1127, 212-225	8
1720	Molecular and supramolecular properties of nitroaromatic thiosemicarbazones: Synthesis, spectroscopy, X-ray structure elucidation and DFT calculations. <b>2017</b> , 1131, 79-86	7
1719	A Hirshfeld surface analysis, crystal structure and physicochemical studies of a new Cd(II) complex with the 2-amino-4-methylpyrimidine ligand. <b>2017</b> , 1128, 378-384	7
1718	Crystal structure and Hirshfeld surface analysis of aqua-bis-(nicotinamide- $\pi$ )-bis-(2,4,6-tri-methyl-benzoato- $\pi$ )-zinc. <b>2017</b> , 73, 1348-1352	3
1717	Structural and computational analysis of intermolecular interactions in a new 2-thiouracil polymorph. <b>2017</b> , 73, 1078-1086	3
1716	(O)-5-[1-Hydroxy-3-(3,4,5-tri-methoxy-phenyl)allylidene]-1,3-di-methyl-pyrimidine-2,4,6-trione: crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 1197-1201	
1715	Crystal structure and Hirshfeld surface analysis of ethyl 5-phenyl-isoxazole-3-carboxylate. <b>2017</b> , 73, 531-534	3
1714	Bis[-2-hydroxy-ethyl,-methyl-dithio-carbamato- $\pi$ ]-4-[[pyridin-4-yl-methylidene)hydrazinylidene)methyl]pyridine- $\pi$ -zinc crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 1458-1464	5

1713	Bis(μ-(1,3-di-phenyl-prop-2-en-1-yl-idene)amino)-ethyl-carbamimido-thioato-κ)zinc(II): crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 1001-1008	6
1712	Synthesis, Crystal Structure and Hirshfeld Topology Analysis of Polymeric Silver(I) Complex with s-Triazine-Type Ligand. <b>2017</b> , 7, 160	1
1711	Synthesis, Crystal Structure and Luminescent Properties of 2D Zinc Coordination Polymers Based on Bis(1,2,4-triazol-1-yl)methane and 1,3-Bis(1,2,4-triazol-1-yl)propane. <b>2017</b> , 7, 354	3
1710	μ-Chlorido-μ-Chlorido-(μ-pyrrolidine-1-carbo-dithioato-κ')tris-[(tri-ethyl-phosphane-κ)Copper(I)]: crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 720-725	3
1709	Formation of Two Kinds of Columnar Crystal Structures of Saddle-Shape Metal Complex [Ni(tmtaa)] Induced by Halogen Substitution. <b>2017</b> , 90, 863-871	
1708	Crystal structure of 4-amino-3-(thio-phen-3-ylmeth-yl)-1,2,4-triazole-5(4)-thione. <b>2017</b> , 73, 1389-1392	1
1707	(μ-Adipato-κ',κ'')bis-[aqua-(benzene-1,2-di-amine-κ)-chlorido-cadmium]: crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 1363-1367	
1706	μ-[1-(5-Bromo-2-hydroxy-phen-yl)ethyl-idene]isonicotinohydrazide monohydrate: crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 630-636	5
1705	Secondary bonding in di-methyl-bis-(morpholine-4-carbodi-thioato-κ)tin(IV): crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 842-848	6
1704	Curved Receptors. <b>2017</b> , 311-328	17
1703	Crystal structure and Hirshfeld analysis of the 4-(di-methyl-amino)-pyridine adduct of 4-meth-oxy-phenyl-borane. <b>2017</b> , 73, 1747-1750	1
1702	A luminescent supramolecular Cu(I)(NH)-sandwiched Cu(pyrazolate) adduct as a temperature sensor. <b>2018</b> , 47, 3679-3683	25
1701	Synthesis and structure elucidation of a novel mixed-ligand Cu(II) Schiff base complex and its catalytic performance for the synthesis of 2-amino-4H-pyrans and tetrahydro-4H-chromenes. <b>2018</b> , 146, 73-80	9
1700	Cyclometalated alkynylgold(III) complexes of 2-phenylpyridine and 2-(p-tolyl)-pyridine [Synthesis, photophysical and electroluminescence properties. <b>2018</b> , 198, 251-259	1
1699	Sonication-assisted synthesis of a new cationic zinc nitrate complex with a tetradentate Schiff base ligand: Crystal structure, Hirshfeld surface analysis and investigation of different parameters influence on morphological properties. <b>2018</b> , 46, 26-35	16
1698	Detailed Analysis of Packing Efficiency Allows Rationalization of Solvate Formation Propensity for Selected Structurally Similar Organic Molecules. <b>2018</b> , 18, 2040-2045	13
1697	Preparation, crystal structure and solution-mediated phase transformation of a novel solid-state form of CL-20. <b>2018</b> , 20, 1553-1563	21
1696	Construction of a Thermally Stable and Highly Energetic Metal-Organic Framework as Lead-Free Primary Explosives. <b>2018</b> , 18, 1896-1902	33

- 1695 Synthesis, X-ray crystal structure, vibrational spectroscopy, DFT calculations, electronic properties and Hirshfeld analysis of (E)-4-Bromo-N'-(2,4-dihydroxy-benzylidene) benzohydrazide. **2018**, 1163, 368-378 23
- 1694 Halides Held by Bifurcated Chalcogen-Hydrogen Bonds. Effect of Cl Contacts on Dimerization of Cl(carbene)Pd Species. **2018**, 57, 3420-3433 56
- 1693 Hydrogen-bonded azaphenacene: a strategy for the organization of  $\pi$ -conjugated materials. **2018**, 6, 3968-3975 11
- 1692 Crystal structures, spectroscopic characterization, and Hirshfeld surface analyses of three constrained cyclam compounds with perchlorate counteranions. **2018**, 1163, 86-93 17
- 1691 Biotransformation, spectroscopic investigation, crystal structure and electrostatic properties of 3,7 $\beta$ -dihydroxyestra-1,3,5(10)-trien-17-one monohydrate studied using transferred electron-density parameters. **2018**, 74, 534-541 3
- 1690 Pb<sup>2+</sup> (X = N, S, I) tetrel bonding interactions in Pb(II) complexes: X-ray characterization, Hirshfeld surfaces and DFT calculations. **2018**, 20, 2812-2821 56
- 1689 Solid-state supramolecular structure formed between the 1-(diaminomethylene)thiourea and mellitic acid. **2018**, 1164, 303-310 4
- 1688 First copper(II)-cyclophosphato complex with macrocyclic N-donor ligand: Single crystal structure elucidation with Hirshfeld surface analysis, optical, electrochemical and antioxidant properties. **2018**, 263, 1-10 3
- 1687 A new six-coordinate organotin(IV) complex of OP[NC<sub>5</sub>H<sub>10</sub>]<sub>3</sub>: A comparison with an analogous five-coordinate complex by means of X-ray crystallography, Hirshfeld surface analysis and DFT calculations. **2018**, 71, 1575-1592 5
- 1686 Magnetic and structural correlations in [Fe(nsald<sub>2</sub>trien)] salts: the role of cation-anion interactions in the spin crossover phenomenon. **2018**, 20, 2465-2475 5
- 1685 7-Methyl-5-[(4-methyl-benzene)-sulfon-yl]-2,5-[1,3]dioxolo[4,5]-indole: crystal structure and Hirshfeld analysis. **2018**, 74, 184-188 11
- 1684 3-Methyl-1-[(1-(4-methyl-pyridin-2-yl)ethylidene)amino]-thio-urea: crystal structure and Hirshfeld surface analysis. **2018**, 74, 256-260 1
- 1683 Crystal structure and Hirshfeld surface analysis of (1-(4-[[2-(4-hydroxy-benzo-yl)hydrazin-1-ylidene]methyl]pyridin-1-ium nitrate. **2018**, 74, 323-327
- 1682 (4-Nitro-phen-yl)methyl 2,3-di-hydro-1-pyrrole-1-carboxyl-ate: crystal structure and Hirshfeld analysis. **2018**, 74, 371-375 1
- 1681 Crystal structure and Hirshfeld surface analysis of 3-cyano-phenyl-boronic acid. **2018**, 74, 441-444 2
- 1680 Synthesis, crystal structure, hirshfeld surface analyses and physical properties of a new hybrid compound: [C<sub>3</sub>N<sub>6</sub>H<sub>8</sub>]<sub>2</sub>PbCl<sub>5</sub>.Cl. **2018**, 123, 97-110 5
- 1679 Water molecule induced reversible single-crystal-to-single-crystal transformation between two trinuclear Fe(II) complexes with different spin crossover behaviour. **2018**, 47, 4307-4314 19
- 1678 A new perfluoromethyl aminoenone derivative and the role of the hydrogen bonding in the intra- and intermolecular interactions. **2018**, 208, 36-47 10

- 1677 5-(1-Aryl-3-(thiophen-2-yl)-1H-pyrazol-4-yl)-1H-tetrazoles: Synthesis, structural characterization, Hirshfeld analysis, anti-inflammatory and anti-bacterial studies. **2018**, 1160, 63-72 18
- 1676 Theoretical investigations of two adamantane derivatives: A combined X-ray, DFT, QTAIM analysis and molecular docking. **2018**, 1159, 233-245 19
- 1675 Polymorphism in Sn(IV)-Tetrapyrrolyl Porphyrins with a Halogenated Axial Ligand: Structural, Photophysical, and Morphological Study. **2018**, 18, 1437-1447 9
- 1674 From Lead(II) Dithiocarbamate Precursors to a Fast Response PbS Positive Temperature Coefficient Thermistor. **2018**, 57, 2132-2140 16
- 1673 Syntheses, crystal structures and Hirshfeld surface analysis of a coordination polymer of Cu(II) chlorido and a tris-octahedral complex of Ni(II) containing isonicotinoylhydrazone blockers. **2018**, 1160, 368-374 7
- 1672 Crystal structure and Hirshfeld surface analysis of aqua-bis-(nicotinamide- $\pi$ )-bis-(2,4,6-tri-methyl-benzoato- $\pi$ )-cadmium(II). **2018**, 74, 246-251 3
- 1671 Synthesis, crystal structure, Hirshfeld surface analysis, spectroscopic studies, electric and dielectric properties of the new Hg(II) complex with N,N-dimethyl-p-toluidine ligand: [C<sub>9</sub>H<sub>14</sub>N]HgCl<sub>3</sub>. **2018**, 24, 2355-2366 3
- 1670 Structural motifs in the Cu(II), Mn(II) and Zn(II) complexes based on N,N,N-donor dipodal or N,N,N,N-donor tripodal ligands obtained in situ: Synthesis, crystal structures and xanthine oxidase inhibition properties. **2018**, 142, 93-104 1
- 1669 Low temperature X-ray structure analyses combined with NBO studies of a new heteroleptic octa-coordinated Holmium(III) complex with N,N,N-tridentate hydrazono-phthalazine-type ligand. **2018**, 1157, 222-229 4
- 1668 Conformational analysis of a supramolecular synthon: a case study of 8-hydroxyquinoline. **2018**, 20, 652-660 6
- 1667 Screening polymorphism in a Ni(II) metal-organic framework: experimental observations, Hirshfeld surface analyses and DFT studies. **2018**, 20, 746-754 55
- 1666 Relationship between the crystal packing and impact sensitivity of energetic materials. **2018**, 20, 837-848 63
- 1665 Self-assembled 3D heterometallic Zn(II)/K(I) metal-organic framework with the fluorite topology. **2018**, 142, 110-114 5
- 1664 Recurrent supramolecular motifs in discrete complexes and coordination polymers based on mercury halides: prevalence of chelate ring stacking and substituent effects. **2018**, 20, 1065-1076 33
- 1663 Redox reactive (RNC)Cu(I) species stabilized in the solid state via halogen bond with I<sub>2</sub>. **2018**, 233, 371-377 33
- 1662 Synthesis, single crystal X-ray, spectroscopic (FT-IR, UV-Vis, fluorescence, <sup>1</sup>H & <sup>13</sup>C NMR), computational (DFT/B3LYP) studies of some imidazole based picrates. **2018**, 1158, 277-285 7
- 1661 Functionalization of Bambusurils by a Thiol-Ene Click Reaction and a Facile Method for the Preparation of Anion-Free Bambus[6]urils. **2018**, 24, 10793-10801 6
- 1660 Two heptacoordinated manganese(II) complexes of giant pentadentate s-triazine bis-Schiff base ligand: Synthesis, crystal structure, biological and DFT studies. **2018**, 479, 275-285 16

1659	Chiral one-dimensional hydrogen-bonded architectures constructed from single-enantiomer phosphoric triamides. <b>2018</b> , 74, 608-617	7
1658	Progressive Cation Triggered Anion Binding by Electron-Rich Scaffold: Case Study of a Neutral Tripodal Naphthyl Thiourea Receptor. <b>2018</b> , 18, 3138-3150	10
1657	Cd(II) Pseudohalide Complexes with N, N'-Bis(3-ethoxysalicylideneimino) 1,3-Diaminopropane: Crystal Structures, Hirshfeld Surface, Antibacterial and Anti-Biofilm Properties. <b>2018</b> , 3, 2912-2925	9
1656	New hybrid of the barbituric acid motif: synthesis, X-ray single crystal, DFT, and Hirshfeld surface analyses. <b>2018</b> , 44, 4213-4225	2
1655	Nonfullerene Electron Transporting Material Based on Naphthalene Diimide Small Molecule for Highly Stable Perovskite Solar Cells with Efficiency Exceeding 20%. <b>2018</b> , 28, 1800346	64
1654	One pot synthesis of two Mn(II) perchlorate complexes with s-triazine NNN-pincer ligand; molecular structure, Hirshfeld analysis and DFT studies. <b>2018</b> , 1164, 344-353	17
1653	Chiral and achiral 1D copper(II) coordination polymers based on glycolato and chelating aromatic diamine ligands. <b>2018</b> , 20, 2455-2464	8
1652	Experimental, Theoretical, Characterization and TD-DFT Analysis of a Complex [Cu(CAP)2Cl2]. <b>2018</b> , 28, 1636-1647	4
1651	Synthesis, X-ray structural, Hirshfeld surface analysis, FTIR, MEP and NBO analysis using DFT study of a 4-chlorobenzylammonium nitrate (C7ClH9N)+(NO3) <sup>-</sup> <b>2018</b> , 1164, 486-492	18
1650	High-Performance Visible-Blind UV Phototransistors Based on n-Type Naphthalene Diimide Nanomaterials. <b>2018</b> , 10, 11826-11836	26
1649	Observation of 3D isostructurality in halogen substituted N -benzoyl- N -phenylbenzamides. <b>2018</b> , 1164, 280-288	
1648	Quantitative investigation of intermolecular interactions in dimorphs of 3-Chloro-N-(2-fluorophenyl)benzamide and 2-Iodo-N-(4-bromophenyl)benzamide. <b>2018</b> , 130, 1	1
1647	Cd(II) and Ni(II) complexes from aroyl hydrazones: Unravelling the intermolecular interactions and electronic, crystal structures through experimental and theoretical studies. <b>2018</b> , 469, 264-279	17
1646	Solid-state supramolecular architectures formed by co-crystallization of melamine and 2-, 3- and 4-fluorophenylacetic acids. <b>2018</b> , 1152, 237-247	6
1645	Mononuclear late first row transition metal complexes of ONO donor hydrazone ligand: Synthesis, characterization, crystallographic insight, in vivo and in vitro anti-inflammatory activity. <b>2018</b> , 1153, 299-310	17
1644	p-halo N4-phenyl substituted thiosemicarbazones: Crystal structure, supramolecular architecture, characterization and bio-assay of their Co(III) and Ni(II) complexes. <b>2018</b> , 1156, 115-126	14
1643	Sonochemical synthesis of a novel nanoscale 1D lead(II) [Pb(L)(I)] coordination Polymer, survey of temperature, reaction time parameters. <b>2018</b> , 42, 320-326	14
1642	Solid-state assembly of 4,4'-bipyridine and proximal p-tert-butylcalix[4]dihydroquinone units** Dedicated to Prof. Jerry L. Atwood on the occasion of his 75th birthday. View all notes. <b>2018</b> , 30, 438-444	

1641	Efficient Optical-to-THz Conversion Organic Crystals with Simultaneous Electron Withdrawing and Donating Halogen Substituents. <b>2018</b> , 6, 1700930	18
1640	Changing Interactions and Conformational Adjustments of N-(Isonicotinylhydrazide)-1,8-naphthalimide by Hydration and Complexation Affect Photophysical Properties. <b>2018</b> , 18, 456-465	23
1639	A comparison of structural and luminescence properties of lead(II) coordination polymers with isomeric thiophenecarboxylate ligands. <b>2018</b> , 471, 446-458	19
1638	Puckering behavior in six new phosphoric triamides containing aliphatic six- and seven-membered ring groups and a database survey of analogous ring-containing structures. <b>2018</b> , 74, 28-41	10
1637	Crystalline packing in pentacene-like organic semiconductors. <b>2018</b> , 20, 63-74	46
1636	Sulfanyl vs sulfonyl, 4,5- vs 3,6- position. How structural variations in phthalonitrile substitution affect their infra-red, crystallographic and Hirshfeld surface analyses. <b>2018</b> , 1155, 310-319	8
1635	Synthesis, Photophysical and Computational Study of Novel Coumarin-based Organic Dyes. <b>2018</b> , 94, 261-276	8
1634	A detailed study of intermolecular interactions, electronic and vibrational properties of the metal complex bis(uracilato)diammine copper(ii) dihydrate. <b>2018</b> , 1155, 424-433	2
1633	Two novel magnesium(II) meso-tetraphenylporphyrin-based coordination complexes: Syntheses, combined experimental and theoretical structures elucidation, spectroscopy, photophysical properties and antibacterial activity. <b>2018</b> , 258, 477-484	21
1632	Coordination of N,O-donor appended Schiff base ligand (H2L1) towards Zinc(II) in presence of pseudohalides: Syntheses, crystal structures, photoluminescence, antimicrobial activities and Hirshfeld surfaces. <b>2018</b> , 1155, 745-757	19
1631	Structure-property relation and third-order nonlinear optical studies of two new halogenated chalcones. <b>2018</b> , 233, 349-360	12
1630	Supramolecular features of 2-(chlorophenyl)-3-[(chlorobenzylidene)-amino]-2,3-dihydroquinazolin-4(1 H)-ones: A combined experimental and computational study. <b>2018</b> , 1155, 78-89	2
1629	Solid-state supramolecular structure of tetrakis(1-(diaminomethylene)thiourea-1-ium) pyromellate. <b>2018</b> , 1155, 443-449	6
1628	Bromobismuthates: Cation-induced structural diversity and Hirshfeld surface analysis of cation-anion contacts. <b>2018</b> , 139, 282-288	25
1627	Weak and strong hydrogen bonds conducting the supramolecular framework of 1-butyl-3-(1-naphthoyl)thiourea: crystal structure, vibrational studies, DFT methods, Pixel energies and Hirshfeld surface analysis. <b>2018</b> , 116, 399-413	9
1626	Influence of insolubility of silver on the Hirshfeld surface analyses and magnetic behavior of La <sub>0.5</sub> Ca <sub>0.1</sub> Ag <sub>0.4</sub> MnO <sub>3</sub> compound. <b>2018</b> , 691, 262-270	9
1625	A combined X-ray crystallography and theoretical study of N-H...OX (X is =P and -C) hydrogen bonds in two new structures with a (C-O)(N)P(=Y) (Y is O and S) skeleton. <b>2018</b> , 74, 1610-1621	5
1624	The Importance of CH...X (X = O, N) Interaction of a New Mixed Ligand Cu(II) Coordination Polymer: Structure, Hirshfeld Surface and Theoretical Studies. <b>2018</b> , 8, 455	28

1623	Molecular Adducts of Isoniazid: Crystal Structure, Electronic Properties, and Hirshfeld Surface Analysis. <b>2018</b> , 59, 1518-1533	8
1622	Hydrogen-bonded Supramolecular Association in Organic Acid-base Pyrimidine Salt and Hirshfeld Surface Analysis. <b>2018</b> , 1083, 012048	1
1621	Neutral host-guest capsular associations by a homologous halophenyl-substituted organic tris-urea receptor series: solid and solution state studies. <b>2018</b> , 42, 19164-19177	6
1620	Stabilization of SF with Glyme-Coordinated Alkali Metal Cations. <b>2018</b> , 57, 14882-14889	10
1619	Synthesis of Mixed-Ligand Nitrile and Carbonyl Isocyanide Complexes of Platinum(II) and Their Reaction with P-Toluenesulfonyl Hydrazide. <b>2018</b> , 88, 2347-2353	1
1618	Packing Structures of CL-20-Based Cocrystals. <b>2018</b> , 18, 7065-7078	31
1617	Crystal structure and Hirshfeld surface analysis and energy frameworks of 1-(2,4-di-methyl-phen-yl)-4-(4-meth-oxy-phen-yl)naphthalene. <b>2018</b> , 74, 939-943	3
1616	Unexpected formation of polymeric silver(I) complexes of azine-type ligand via self-assembly of Ag-salts with isatin oxamohydrazide. <b>2018</b> , 5, 180434	4
1615	Solvent Effects on the Spin-Transition in a Series of Fe(II) Dinuclear Triple Helicate Compounds. <b>2018</b> , 8, 376	6
1614	High-Throughput Pressure-Dependent Density Functional Theory Investigation of Herringbone Polycyclic Aromatic Hydrocarbons: Part 2. Pressure-Dependent Electronic Properties. <b>2018</b> , 122, 23828-23844	8
1613	Multicomponent Supramolecular Assemblies of Melamine and $\pi$ -Hydroxycarboxylic Acids: Understanding the Hydrogen Bonding Patterns and Their Physicochemical Consequences. <b>2018</b> , 18, 6786-6800	16
1612	Synthesis and Characterization of Heterometallic Iron-Uranium Complexes with a Bidentate N-Donor Ligand (2,2'-Bipyridine or 1,10-Phenanthroline). <b>2018</b> , 57, 13318-13329	8
1611	High-Throughput Pressure-Dependent Density Functional Theory Investigation of Herringbone Polycyclic Aromatic Hydrocarbons: Part 1. Pressure-Dependent Structure Trends. <b>2018</b> , 122, 23815-23827	7
1610	Noncovalent Interactions Involving Iodofluorobenzenes: The Interplay of Halogen Bonding and Weak $\text{I}(\text{O})\cdots\pi$ Holearene Interactions. <b>2018</b> , 18, 7641-7654	49
1609	Crystal structure and Hirshfeld surface analysis of ()-4-(4-hydroxy-benzyl-idene)-3-methyl-isoxazol-5(4)-one. <b>2018</b> , 74, 926-930	2
1608	Systematic Modulation of the Supramolecular Gelation Properties of Bile Acid Alkyl Amides. <b>2018</b> , 24, 18676-18681	4
1607	Synthesis, crystal structure, Hirshfeld surface analysis and IR investigation of $\text{Hf}(\text{SeO}_4)_2(\text{H}_2\text{O})_4$ . <b>2018</b> , 17-18, 312-320	5
1606	A Stable Crown Ether Complex with a Noble-Gas Compound. <b>2018</b> , 130, 12628-12632	6

- 1605 X-ray crystal structure, Hirshfeld surface analysis and NMR study of novel copper(I) alkyl dithio- and perthio-carboxylates. **2018**, 17-18, 205-218
- 1604 Revealing the roles of solvation in D-mannitol's polymorphic nucleation. **2018**, 20, 7435-7445 21
- 1603 X-ray crystal structure, Hirshfeld surface analysis and DFT computations of a hydroxyphosphine oxide derivative [(4-hydroxy-2-methylpentan-2-yl)diphenylphosphine oxide]. **2018**, 17-18, 287-301
- 1602 Structural and Electronic Effects Due to Fluorine Atoms on Dibenzotetraaza-Annulenes Complexes. **2018**, 3, 10074-10083 2
- 1601 Structural characterization and Hirshfeld surface analysis of a Co complex with imidazo[1,2-]pyridine. **2018**, 74, 600-606 30
- 1600 Conformational trimorphism of bis(2,6-dimesitylphenyl)ditelluride. **2018**, 233, 707-721
- 1599 Physico-chemical characterization, Hirshfeld surface analysis and opto-electric properties of a new hybrid material: Tris (2-amino-5-chloropyridinium) hexachlorobismuthate(III). **2018**, 1173, 439-447 18
- 1598 Synthesis and structure of a cobalt(III) complex containing pendant Schiff base ligand: Exploration of its catechol oxidase and phenoxazinone synthase like activity. **2018**, 482, 23-33 18
- 1597 Crystal structure, hydrogen bonding and Hirshfeld surface analysis of 2-amino-4-methoxy-6-methyl-pyrimidinium 4-chloro-benzoate. **2018**, 74, 656-659 2
- 1596 Investigations based on non-covalent interactions in 1-(4-chloromethylbenzoyl)-3-(4,6-di-substituted pyrimidine-2-yl)thioureas: Synthesis, characterizations and quantum chemical calculations. **2018**, 1169, 85-95 8
- 1595 Synthesis, crystal structure and Hirshfeld surface analysis of a benzoxazole derivative [2-[2-(4-Methylphenyl)ethenyl]-1,3-benzoxazole]. **2018**, 15-16, 161-169 1
- 1594 Synthesis, crystal structure, Hirshfeld surface and DFT studies of ([Cu(3-ptp) 2 (p-TS) 2 ]) from decomposition of tosylhydrazone. **2018**, 1169, 59-67 13
- 1593 X-ray crystal structure, Hirshfeld surface analysis, thermal stability and photophysical properties of some symmetrical trans- $\beta,\beta'$ -bis(diphenylphosphoryl)- and  $\beta,\beta'$ -bis(diphenylphosphorothioyl)cycloalkanones. **2018**, 1171, 279-293 4
- 1592 Ligation-Enhanced  $\pi$ -Hole $\cdots\pi$  Interactions Involving Isocyanides: Effect of  $\pi$ -Hole $\cdots\pi$  Noncovalent Bonding on Conformational Stabilization of Acyclic Diaminocarbene Ligands. **2018**, 57, 6722-6733 43
- 1591 Synthesis, characterization and crystal structure of 2-chloroethyl(methylsulfonyl)methanesulfonate. **2018**, 42, 11073-11084 7
- 1590 Synthesis, crystal structure studies and Hirshfeld surface analysis of 6-chloro-7-hydroxy-4-methyl-2H-chromen-2-one. **2018**, 15-16, 134-142 3
- 1589 Quantifying intermolecular interactions for isoindole derivatives: substituent effect vs. crystal packing. **2018**, 233, 675-687 4
- 1588 Yellow-Colored Electro-Optic Crystals as Intense Terahertz Wave Sources. **2018**, 28, 1801143 21



1587	Structural features of 7-methoxy-5-methyl-2-(pyridin-3-yl)-11,12-dihydro-5,11-methano[1,2,4]triazolo[1,5-c][1,3,5]benzoxadiazocine: Experimental and theoretical (HF and DFT) studies, surface properties (MEP, Hirshfeld). <b>2018</b> , 1168, 280-290	31
1586	Structure-Directing Weak Interactions with 1,4-Diodotetrafluorobenzene Convert One-Dimensional Arrays of [MII(acac) <sub>2</sub> ] Species into Three-Dimensional Networks. <b>2018</b> , 18, 3626-3636	33
1585	Crystal structure and Hirshfeld surface analysis of -(2-hydroxy-naphthalen-1-yl)(3-methyl-phen-yl)meth-yl]acetamide. <b>2018</b> , 74, 1002-1005	1
1584	Synthesis and crystal structures of new phosphoric triamides: study of intermolecular interactions by semi-empirical calculations and Hirshfeld surface analysis. <b>2018</b> , 149, 1759-1776	6
1583	New 3D Supramolecular Ag(I) Coordination Polymer Crystal Containing 2-Quinaldic Acid Radical Biological Ligand: Crystal Structure and Anticancer Activity. <b>2018</b> , 53, 1800065	23
1582	A Stable Crown Ether Complex with a Noble-Gas Compound. <b>2018</b> , 57, 12448-12452	16
1581	Optical nonlinearity and charge transfer analysis of 4-[(E)-2-(2,4,6-Trinitrophenyl) ethylidene] benzonitrile adsorbed on silver nanoparticles: Computational and experimental investigations. <b>2018</b> , 107, 454-467	3
1580	Organic co-crystals of 1,3-bis(4-pyridyl)azulene with a series of hydrogen-bond donors. <b>2018</b> , 20, 4463-4484	3
1579	Spontaneous resolution of a chiral-at-metal pseudo-tetrahedral Schiff-base zinc complex to a racemic conglomerate with CH <sub>2</sub> O organized 41- and 43-helices. <b>2018</b> , 20, 4724-4734	15
1578	Synthesis, structural characterization, DFT calculations and Hirshfeld surface analysis of (R)-2-((S)-2((S)-hydroxy(ferrocenyl)methyl)aziridin-1-yl)butan-1-ol. <b>2018</b> , 1173, 33-41	2
1577	Evaluation of N-H...S and N-H...O interactions in O,O'-diethyl N-(2,4,6-trimethylphenyl)thiophosphate: a combination of X-ray crystallographic and theoretical studies. <b>2018</b> , 74, 847-855	9
1576	Crystal structure and Hirshfeld surface analysis of ()-3-(2-chloro-4-fluoro-phen-yl)-1-(2,5-di-chloro-thio-phen-3-yl)prop-2-en-1-one. <b>2018</b> , 74, 1134-1137	2
1575	Crystal structure analysis of [5-(4-methoxy-phen-yl)-2-methyl-2,1,2,3-triazol-4-yl](thio-phen-2-yl)methanone. <b>2018</b> , 74, 1178-1181	6
1574	The effects of altering reaction conditions in synthesis of a novel lead(II) 2D coordination polymer as well as in achieving the same morphologies of lead(II)oxide micro-nano structures via solid-state process. <b>2018</b> , 154, 443-456	8
1573	Solvated and Ferroelectric Phases of the Charge Transfer Co-Crystal TMB-TCNQ. <b>2018</b> , 18, 5592-5599	7
1572	X-ray crystal structure, Hirshfeld surface analysis and DFT study of some cis-5-hydroxy-2-phosphono-2,5-dihydrofurans. <b>2018</b> , 17-18, 95-110	0
1571	Copper(II) complexes of 7-amino-2-methylchromone and 7-aminoflavone: Magneto-structural, spectroscopic and DFT characterization. <b>2018</b> , 153, 181-196	4
1570	Theoretical Investigations on Molecular Packing Motifs and Charge Transport Properties of a Family of Trialkylsilylethynyl-Modified Pentacenes/Anthradithiophenes. <b>2018</b> , 122, 18880-18894	12

- 1569 Intra-/Intermolecular Bifurcated Chalcogen Bonding in Crystal Structure of Thiazole/Thiadiazole Derived Binuclear (Diaminocarbene)PdII Complexes. **2018**, 8, 112 26
- 1568 Structural Characterized Homotrinary ZnII Bis(Salamo)-Based Coordination Compound: Hirshfeld Surfaces, Fluorescent and Antimicrobial Properties. **2018**, 8, 259 9
- 1567 Evolution of Interatomic and Intermolecular Interactions and Polymorphism of Melamine at High Pressure. **2018**, 8, 265 7
- 1566 Crystal Engineering of Naturally Occurring Seselin To Obtain Cocrystal with Enhanced Anti-Leishmanial Activity, Hirshfeld Surface Analysis, and Computational Insight. **2018**, 18, 4628-4636 8
- 1565 Synthesis, Crystal Structure and DFT Studies of a New Dinuclear Ag(I)-Malonamide Complex. **2018**, 23, 4
- 1564 Exploring weak intermolecular interactions in thiocyanate-bonded Zn(ii) and Cd(ii) complexes with methylimidazole: crystal structures, Hirshfeld surface analysis and luminescence properties.. **2018**, 8, 23891-23902 20
- 1563 Structural and electronic properties of 5,5'-Hydrazinebistetrazole under high pressure: A DFT study. **2018**, 377, 012107 1
- 1562 Supramolecular framework of conjugated nitro-alkenes: Crystallographic and hirshfeld surface scan. **2018**, 1173, 964-973 3
- 1561 Hydrogen Bond Donor/Acceptor Ratios of the Coformers: Do They Really Matter for the Prediction of Molecular Packing in Cocrystals? The Case of Benzamide Derivatives with Dicarboxylic Acids. **2018**, 18, 5254-5269 11
- 1560 Racemic mefloquinium chloro-difluoro-acetate: crystal structure and Hirshfeld surface analysis. **2018**, 74, 895-900 3
- 1559 Interaction leading to an inversion-symmetric complex pair of  $\pi$  and  $\pi$  bis[N-2-(R-pyridyl)-2-oxo-1-naphthalidiminato- $\pi$ N,O]zinc(II). **2018**, 482, 935-942 10
- 1558 Exploring a solvated dimer of Gefitinib: a quantitative analysis. **2018**, 74, 944-950 8
- 1557 Erratum to Molecular structure, spectroscopic properties, and Hirshfeld surface analysis of chlorobis(N-methyl-1,3-propanediamine)copper(II) tetrafluoroborate and azidobis(2,2-dimethyl-1,3-propanediamine)copper(II) azide[J. Mol. Struct. 1154 (2018) 338-347]. **2018**, 1168, 329
- 1556 Structural and energetic aspects of adamantane and memantine derivatives of sulfonamide molecular crystals: experimental and theoretical characterisation. **2018**, 20, 3476-3489 14
- 1555 A novel potential anticancer chalcone: Synthesis, crystal structure and cytotoxic assay. **2018**, 1168, 309-315 7
- 1554 Quantifying conventional  $\pi$ - $\pi$  (aryl) and unconventional  $\pi$ - $\pi$  (chelate) interactions in dinuclear Cu(II) complexes: experimental observations, Hirshfeld surface and theoretical DFT study. **2018**, 42, 10202-10213 59
- 1553 High-pressure behavior and Hirshfeld surface analysis of nitrogen-rich materials: triazido-s-triazine (TAT) and triazido-s-heptazine (TAH). **2018**, 53, 15977-15985 4
- 1552 Modulating the DNA cleavage ability of copper(II) Schiff bases through ternary complex formation. **2018**, 42, 15170-15183 8

1551	An anion receptor that facilitates transmembrane proton-anion symport by deprotonating its sulfonamide N-H proton. <i>Chemical Communications</i> , <b>2018</b> , 54, 10351-10354	5.8	9
1550	-[6-Methoxy-pyridin-2-yl]-1-(pyridin-2-ylmethyl)-1-pyrazole-3-carboxamide: crystal structure and Hirshfeld surface analysis. <b>2018</b> , 74, 1254-1258		
1549	Theoretical and experimental approach to the investigation of hyperpolarizability and charge transfer characteristics of NLO active 2,3,4,4',5-pentamethoxy chalcone with silver atoms adsorbed. <b>2018</b> , 84, 409-421		10
1548	Triethylphosphine as a molecular gear - phase transitions in ferrocenyl-acetylide-gold(I). <b>2018</b> , 74, 427-435		2
1547	Undeca-carbon-yl[(4-methyl-sulfanylphenyl)di-phenyl-phosphane]triruthenium(0): crystal structure and Hirshfeld surface analysis. <b>2018</b> , 74, 791-795		
1546	A new high-spin iron(III) bis(aqua) complex with the meso-tetra(para-chlorophenyl)porphyrin: X-ray crystallography, Hirshfeld surface analysis, magnetic, EPR and electrochemical properties. <b>2018</b> , 44, 7259-7276 <sup>5</sup>		
1545	Synthesis, single crystal, structure and Hirshfeld surface analysis of (E)-4-toluic-N'-(2,4-dihydroxy-benzylidene) benzohydrazide. <b>2018</b> , 17-18, 169-177		7
1544	Supramolecular architecture in azaheterocyclic phosphonates. III. Structures of an ethyl phosphonamidate and an ethyl phosphonate. <b>2018</b> , 74, 907-916		
1543	Synthesis, physicochemical and theoretical studies on new rhodium and ruthenium dimers. Relationship between structure and cytotoxic activity. <b>2018</b> , 154, 263-274		5
1542	The "Wanderlust" of MeSi groups in rare-earth triple-decker complexes: a combined experimental and computational study. <i>Chemical Communications</i> , <b>2018</b> , 54, 10280-10283	5.8	7
1541	Unusual constructions of two Salamo-based copper(II) complexes. <b>2018</b> , 203, 56-64		46
1540	Structural and spectroscopic characterization of bis[1-(diaminomethylene)thiourea-1-ium] naphthalene-1,5-disulfonate. <b>2018</b> , 1171, 411-419		
1539	Synthesis, characterisation and structure determination of 3-[(1Z)-{2-[bis((2-methylphenyl)methyl)sulfanyl]methylidene}hydrazin-1-ylidene)methyl]benzene-1,2-diol. <b>2018</b> , 1171, 650-657		2
1538	Crystal structures and Hirshfeld surface analyses of (-hexyl-methyl-dithio-carbamato- $\pi$ )triphenyl-tin(IV) and [-methyl-(2-phenyl-ethyl)-dithio-carbamato- $\pi$ ]tri-phenyl-tin(IV). <b>2018</b> , 74, 630-637		2
1537	Polymorphism of Sildenafil: A New Metastable Desolvate. <b>2018</b> , 18, 3740-3746		13
1536	Complete Set of Elastic Moduli of a Spin-Crossover Solid: Spin-State Dependence and Mechanical Actuation. <b>2018</b> , 140, 8970-8979		42
1535	Five benzoic acid derivatives: Crystallographic study using X-ray powder diffraction, electronic structure and molecular electrostatic potential calculation. <b>2019</b> , 1175, 185-194		8
1534	Synthesis, crystal structure, infrared spectroscopy, thermal analysis and Hirshfeld surface analysis of a new hemihydrate of [Zn (H <sub>2</sub> O) 6][{(CH <sub>2</sub> ) <sub>6</sub> N <sub>4</sub> }ZnCl <sub>3</sub> ] <sub>2</sub> ·0.5H <sub>2</sub> O. <b>2019</b> , 1176, 165-180		2

1533	Efficient Gap-Free Broadband Terahertz Generators Based on New Organic Quinolinium Single Crystals. <b>2019</b> , 7, 1900953	9
1532	A novel hybrid iron fluoride based on 8-hydroxyquinoline: Crystal structure, thermal decomposition, spectroscopic characterization, and magnetic properties. <b>2019</b> , 496, 119033	2
1531	Crystal Structures and Characteristics of Hirshfeld Surfaces of Co(II) $\beta$ -iminoketonate Derivatives. <b>2019</b> , 60, 1052-1061	3
1530	Role of lone pair- $\pi$ interaction and halogen bonding in the crystal packing of 1,2,4-oxadiazole derivatives. <b>2019</b> , 1197, 742-752	3
1529	Synthesis and characterization of a new 4-styrylpyridine based square planar copper(II) complex: exploration of phenoxazinone synthase-mimicking activity and DFT study. <b>2019</b> , 72, 2362-2375	4
1528	Synthesis, structure and Hirshfeld analysis of the potent antimicrobial [Ag(4-bromopyrazole) <sub>2</sub> ClO <sub>4</sub> ] complex. <b>2019</b> , 171, 323-329	2
1527	Enol-imino-Keto-enamine Tautomerism in a Diazepine Derivative: How Decisive Are the Intermolecular Interactions in the Equilibrium?. <b>2019</b> , 84, 11042-11053	13
1526	Structural variety of clofaziminium salts: effect of the counter-ion on clofaziminium conformation and crystal packing. <b>2019</b> , 75, 674-686	3
1525	Polymorphism and resulting luminescence properties of 1-acetylpyrene. <b>2019</b> , 21, 5845-5852	4
1524	Synthesis, characterization, DFT calculations, electric and dielectric properties of (C <sub>6</sub> H <sub>10</sub> (NH <sub>3</sub> ) <sub>2</sub> )CdCl <sub>4</sub> ·H <sub>2</sub> O organic-inorganic hybrid compound. <b>2019</b> , 1198, 126887	1
1523	Exploring the different environments effect of piperine via combined crystallographic, QM/MM and molecular dynamics simulation study. <b>2019</b> , 92, 280-295	5
1522	Flexible control of excited state transition under pressure/temperature: distinct stimuli-responsive behaviours of two ES IPT polymorphs. <b>2019</b> , 3, 2128-2136	8
1521	The (Current) Acridine Solid Form Landscape: Eight Polymorphs and a Hydrate. <b>2019</b> , 19, 4884-4893	9
1520	Charge Transfer Versus Arene- $\pi$ -fluoroarene Interactions in Modulation of Optical and Conductivity Properties in Cocrystals of 2,7-Di-tert-butylpyrene. <b>2019</b> , 123, 18198-18206	17
1519	Synthesis, Crystal Structure, Spectroscopic Properties, and Hirshfeld Surface Analysis of Diaqua [3,14-dimethyl-2,6,13,17 tetraazatricyclo(16.4.0.07,12)docosane]copper(II) Dibromide. <b>2019</b> , 9, 336	9
1518	Halogenated imidazo[1,5-a]pyridines: chemical structure and optical properties of a promising luminescent scaffold. <b>2019</b> , 171, 107713	12
1517	Hunting for advanced high-energy-density materials with well-balanced energy and safety through an energetic host-guest inclusion strategy. <b>2019</b> , 7, 19248-19257	40
1516	Exploring concomitant/conformational dimorphism in a difluoro-substituted phosphoramidate derivative. <b>2019</b> , 75, 451-461	5

1515	The heteroscorpionate ligand 2,2-bis(3,5-dimethylpyrazol-1-yl)-1,1-diphenylethanol and an easy preparation of its tungsten complex. <b>2019</b> , 75, 996-1001		
1514	Synthesis, structural characterization, Hirshfeld surface analysis, antimicrobial activity, and DNA cleavage studies of (Z)-4-methyl-N'-(phenyl(pyridin-2-yl)methylene)benzenesulfonohydrazide and its Co(II), Ni(II) and Zn(II) complexes. <b>2019</b> , 1196, 760-770		3
1513	A quantitative study of weak noncovalent interactions in two pyridine isomers containing nitrile and thiophene moieties: a combined X-ray and theoretical investigation. <b>2019</b> , 131, 1		4
1512	Synthesis, crystal structure, electrochemiluminescence property of a novel cadmium (II) coordination polymer possessing 4-cyanopyrazole. <b>2019</b> , 107, 107489		1
1511	Design and construction of Zn(II) coordination polymers made by pincer type pyridine-hydrazine based ligands. <b>2019</b> , 1197, 555-563		6
1510	Drug-drug salts of mefenamic acid/tolfenamic acid and piperazine to improve physicochemical properties for potential veterinary use. <b>2019</b> , 21, 5284-5291		3
1509	Crystal Structure, Stability and Desolvation of the Solvates of Sorafenib Tosylate. <b>2019</b> , 9, 367		11
1508	Synthesis, structure and density functional theory calculations of a novel photoluminescent trisarylborane-bismuth(III) complex. <b>2019</b> , 34, 731-738		1
1507	A comprehensive study on crystal structure of a novel sulfonamide-dihydroquinolinone through experimental and theoretical approaches. <b>2019</b> , 25, 205		5
1506	Racemic Salts and Solid Solutions of Enantiomers of the Antihypertensive Drug Carvedilol. <b>2019</b> , 19, 4498-4509		6
1505	A new ferroelastic hybrid material with a large spontaneous strain: (MeNOH)[ZnCl]. <i>Chemical Communications</i> , <b>2019</b> , 55, 8983-8986	5.8	23
1504	Experimental and molecular modeling study of a novel arylsulfonamide chalcone. <b>2019</b> , 25, 208		1
1503	The direct synthesis of a substituted naphthopentathiepin for selective Co <sup>2+</sup> ion recognition in aqueous solution. <b>2019</b> , 95, 135-145		2
1502	Metal-4,4'-azobis(3,5-dimethyl-1H-pyrazole) Complexes with Seven- and Nine-membered Hydrogen-bonded Rings Originating from the Pyrrolic NH Function. <b>2019</b> , 645, 893-899		1
1501	Crystal structures and supramolecular architectures of ONO donor hydrazone and solvent exchangeable dioxidomolybdenum(VI) complexes derived from 3,5-diiodosalicylaldehyde-4-methoxybenzoylhydrazone: Hirshfeld surface analysis and interaction energy calculations. <b>2019</b> , 170, 749-761		8
1500	Solid-Liquid Phase Equilibrium and Thermodynamic Analysis of N,N'-Diethylthiourea in Different Solvent Systems. <b>2019</b> , 64, 6031-6040		12
1499	Synthesis, characterization crystal and molecular structure studies of 5-(3-Methylbenzoyl)-4-methyl-1,3,4,5-tetrahydro-2H-1,5-benzodiazepin-2-one: Hirshfeld surface analysis and DFT calculations. <b>2019</b> , 24, 100292		1
1498	Indirect influence of alkyl substituent on sigma-hole interactions: The case study of antimony(III) diphenyldithiophosphates with covalent Sb-S and non-covalent Sb $\cdots$ S pnictogen bonds. <b>2019</b> , 173, 114126		15

- 1497 Ordered and Plastic Crystals in the Complex Polymorphism of Pinanediol. **2019**, 19, 6127-6135 6
- 1496 Synthesis, characterization, crystal structure and hirshfeld surface analysis of alkyl substituted N,4-diphenyl thiazole-2-amine.. **2019**, 24, 100297 1
- 1495 Kinetics study and Hirshfeld surface analysis for atorvastatin calcium trihydrate and furosemide system. **2019**, 682, 178408 4
- 1494 Synthesis, crystal structure and studies of physical parameters of novel compound N-(2,6-dichlorophenyl)-4-(naphthalen-2-yl)-1,3-thiazol-2-amine. **2019**, 24, 100286
- 1493 In situ crystallization of 2,2-dimethoxypropane and dimethyldimethoxysilane: hunting for Group 14 isomorphism. **2019**, 29, 531-533 3
- 1492 Crystal and molecular structures of boldenone and four boldenone steroid esters. **2019**, 234, 671-683 10
- 1491 Fluorinated Organic Electro-Optic Quinolinium Crystals for THz Wave Generation. **2019**, 7, 1801495 8
- 1490 Anisotropic electrical and optical studies of organic biphenyl single crystal grown by modified Czochralski technique. **2019**, 30, 3909-3920 3
- 1489 The synergistic co-operation of N-H...O=P hydrogen bonds and C-H...OX weak intermolecular interactions (X is =P or -C) in the (CHO)P(O)(NH-NHCF) amidophosphoester: a combined X-ray crystallographic and theoretical study. **2019**, 75, 1424-1433 0
- 1488 New Insights into Photochromic Properties of N-Salicylideneaniline Derivatives Using a Cocrystal Engineering Approach. **2019**, 19, 5544-5556 4
- 1487 Bromide and Tribromide 4-Cyanobenzene-Ethylenedithio-Tetrathiafulvalene Radical Salts by Chemical and Electrochemical Routes. **2019**, 19, 5768-5775 4
- 1486 Relative stability of the cis and trans isomers of octahedral cobalt(III) complexes of the type [Co(N2O2)X2] with tetradentate salen type Schiff bases: a combined theoretical and experimental study. **2019**, 21, 6026-6037 6
- 1485 Synthesis and characterization of mixed-ligand Zn(II) and Cu(II) complexes including polyamines and dicyano-dithiolate(2-): In vitro cytotoxic activity of Cu(II) compounds. **2019**, 498, 119098 12
- 1484 Crystal Engineering of 1-Halopolyynes by End-Group Manipulation. **2019**, 19, 6542-6551 3
- 1483 Statistical Prevalence versus Energetic Contributions of F...F, F...H, and F...C Intermolecular Interactions in 4-Trifluorotoluenesulfonamide Crystals. **2019**, 19, 6296-6307 1
- 1482 Molecular Simulation Approaches for the Prediction of Unknown Crystal Structures and Solubilities of (R)- and (R,S)-Crizotinib in Organic Solvents. **2019**, 19, 5882-5895 7
- 1481 A Comprehensive Topological Analysis on a New Bromine-Chalcone with Potential Nonlinear Optical Properties. **2019**, 123, 8632-8643 2
- 1480 A low molecular weight OLED material: 2-(4-((2-hydroxyethyl)(methyl)amino)benzylidene)malononitrile. Synthesis, crystal structure, thin film morphology, spectroscopic characterization and DFT calculations.. **2019**, 9, 28704-28717 3

1479	Versatile solid forms of boscalid: insight into the crystal structures and phase transformations. <b>2019</b> , 21, 6838-6849	4
1478	Azido bridged binuclear copper(II) Schiff base compound: synthesis, structure and electrical properties. <b>2019</b> , 43, 16255-16263	3
1477	Crystal structure and evaluating C H $\pi$ (aryl/chelate) interactions in bis(2-(((2-hydroxyethyl)imino)-methyl)-4,6-diiodophenolato)-palladium(II) Schiff base complex derived from (E)-2-(((2-hydroxyethyl)imino)methyl)-4,6-diiodophenol. <b>2019</b> , 498, 119118	2
1476	A new luminescent organic-inorganic hybrid material based on cadmium iodide. <b>2019</b> , 109, 107572	2
1475	Synthesis, structure and antiproliferative and optical activities of two new biphenyl-derived Schiff bases. <b>2019</b> , 75, 97-106	3
1474	Thiocyanato-metal(II) and azido-cobalt(III) complexes with hydroxymethylpyridines. <b>2019</b> , 161, 309-316	6
1473	Origin of the Immiscibility of Alkanes and Perfluoroalkanes. <b>2019</b> , 141, 3489-3506	22
1472	Structural and Electronic Origin of Bis-Lactam-Based High-Performance Organic Thin-Film Transistors. <b>2019</b> , 11, 8301-8309	9
1471	Intermolecular head-to-head interaction of carbonyl groups in bicyclic hydrogen-bonded synthon based on $\beta$ -hydroxy ketones. <b>2019</b> , 21, 1587-1599	12
1470	Synthesis, structure of 7-oxa-1-azabicyclo[2.2.1]heptane derivative obtained from sugar nitron and analysis of its conformational variety. <b>2019</b> , 1183, 14-23	
1469	Separation or combination of non-covalently linked partners provides polymorphs of N-(aryl)-2-(propan-2-ylidene)hydrazine carbothioamides. <b>2019</b> , 21, 1397-1406	4
1468	The Phase Transformation and Formation Mechanism of Isostructural Solvates: A Case Study of Azoxystrobin. <b>2019</b> , 19, 1550-1558	9
1467	Theoretical study of synergetic effect between halogenation and pyrazine substitutions on transport properties of silylethynylated pentacene. <b>2019</b> , 43, 3583-3600	5
1466	Synthesis, Single Crystal X-ray Structure, DFT Computations, Hirshfeld Surface Analysis and Molecular Docking Simulations on (((1E)-1-(1,3-Benzodioxol-5-yl)-3-(1H-imidazol-1-yl)propylidene]amino)oxy)(furan-2-yl)methanone: A New Antifungal Agent. <b>2019</b> , 9, 25	4
1465	Recognition of the Hole donor ability of iodopentafluorobenzene as conventional Hole donor for crystal engineering involving halogen bonding. <b>2019</b> , 21, 616-628	28
1464	New rhenium-tricarbonyl complexes bearing halogen-substituted bidentate ligands: structural, computational and Hirshfeld surfaces studies. <b>2019</b> , 21, 77-93	9
1463	Modulation of coordination in pincer-type isonicotinohydrazone Schiff base ligands by proton transfer. <b>2019</b> , 21, 108-117	26
1462	Structure determination of fatty acid ester biofuels via in situ cryocrystallisation and single crystal X-ray diffraction. <b>2019</b> , 21, 41-52	5

1461	Preparation, spectral properties and structure of bis(salicylato)bis(benzimidazole)-copper(II) complexes with two different benzimidazole spatial orientation. <b>2019</b> , 170, 86-94	1
1460	An investigation of supramolecular synthons in 1,2,4-triazole-3(4H)-thione compounds. X-ray crystal structures, energetic and Hirshfeld surface analysis. <b>2019</b> , 1195, 796-806	13
1459	Triarylborane-Based Helical Donor-Acceptor Compounds: Synthesis, Photophysical, and Electronic Properties. <b>2019</b> , 25, 10845-10857	18
1458	Enhanced $\pi$ -back-donation resulting in the trans labilization of a pyridine ligand in an N-heterocyclic carbene (NHC) Pd precatalyst: a case study. <b>2019</b> , 75, 941-950	7
1457	Rhodium(III) complexes with isoquinoline derivatives as potential anticancer agents: in vitro and in vivo activity studies. <b>2019</b> , 48, 11469-11479	16
1456	Novel white light emitting dysprosium oxalate nanocrystals: Competing luminescence quenching by the features of Dy-Oxalate layered structure. <b>2019</b> , 804, 252-261	8
1455	High Energy Explosive with Low Sensitivity: A New Energetic Cocrystal Based on CL-20 and 1,4-DNI. <b>2019</b> , 19, 4476-4482	38
1454	Synthesis, photophysical and electronic properties of tetra-donor- or acceptor-substituted -perylene displaying four reversible oxidations or reductions. <b>2019</b> , 10, 7516-7534	26
1453	Experimental study and DFT calculation for the strength of intermolecular interactions in Schiff base with the phenylarsonic acid scaffold. <b>2019</b> , 1196, 306-322	5
1452	Synthesis, Crystal Structure, and Biological Evaluation of Fused Thiazolo[3,2-]Pyrimidines as New Acetylcholinesterase Inhibitors. <b>2019</b> , 24,	5
1451	Cocrystals of Gallic Acid with Urea and Propionamide: Supramolecular Structures, Hirshfeld Surface Analysis, and DFT Studies. <b>2019</b> , 54, 1900016	9
1450	The synthesis of 3-ethyl-5-methyl-2,6-diarylpiperidin-4-on-1-ium picrates and their spectral, XRD and theoretical studies. <b>2019</b> , 43, 11003-11014	6
1449	The crystal structures and Hirshfeld surface analysis of '""-(1,1')-[[methyl-enebis(-oxy)]bis-(6-bromo-3,1-phenyl-ene)]bis-(methan-yl-ylidene))bis-(isonicotinohydrazide) dihydrate and	
1448	'""-(1,1')-[[butane-1,4-diybis(-oxy)]bis-(2,1-phenyl-ene)]bis-(methan-yl-ylidene))bis-(isonicotino-hydrazide) Interplay of weak noncovalent interactions in two conjugated positional isomers: A combined X-ray, optical properties and theoretical investigation. <b>2019</b> , 1195, 32-42	8
1447	A highly sensitive and selective fluorescent "off-on-off" relay chemosensor based on a new bis(salamo)-type tetraoxime for detecting Zn and CN. <b>2019</b> , 222, 117209	80
1446	Synthesis, crystal structure, Hirshfeld surface analysis and dielectric properties of a new centrosymmetric hybrid compound (C <sub>4</sub> H <sub>12</sub> NO <sub>3</sub> )CdCl <sub>3</sub> ·H <sub>2</sub> O. <b>2019</b> , 170, 695-704	2
1445	Crystal Solvates of Energetic 2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane Molecule with [bmim]-Based Ionic Liquids. <b>2019</b> , 19, 3660-3669	8
1444	Introducing pyridyl into electron transport materials plays a key role in improving electron mobility and interface properties for inverted perovskite solar cells. <b>2019</b> , 7, 16304-16312	6



1443	Solvent effect on neutral Co (II) complexes of paeonol derivative Qualitative and quantitative studies from energy frame work and Hirshfeld surface analysis. <b>2019</b> , 1196, 119-131		5
1442	Heat-Induced Polymorphic Transformation Facilitating the Low Impact-Sensitivity of 2,2-Dinitroethylene-1,1-diamine (FOX-7). <b>2019</b> , 123, 16014-16022		16
1441	Halogen bonding-assisted formation of one-dimensional polybromideBromotellurate (2-ClPyH) <sub>2</sub> {[TeBr <sub>6</sub> ](Br <sub>2</sub> )}. <b>2019</b> , 72, 1890-1898		4
1440	Synthesis, crystal structure and Hirshfeld surface analysis of a new 0D nanostructured [[Ar-Cl]tetra-azo-S] <sub>2</sub> Hg coordination supramolecular compound derived from phenyl isothiocyanate ligand. <b>2019</b> , 72, 1671-1682		2
1439	Efficient modulation of photoluminescence by hydrogen bonding interactions between inorganic [MnBr] anions and organic cations. <i>Chemical Communications</i> , <b>2019</b> , 55, 7303-7306	5.8	64
1438	Field-Induced Single-Ion Magnetic Behavior in Two Mononuclear Cobalt(II) Complexes. <b>2019</b> , 14, 2620-2628		6
1437	4-(4-Bromophenyl)thiazol-2-amine: Crystal structure determination, DFT calculations, visualizing intermolecular interactions using Hirshfeld surface analysis, and DNA binding studies. <b>2019</b> , 32, e3968		6
1436	Synthesis, Molecular and Supramolecular Structures of New Cd(II) Pincer-Type Complexes with s-TriazineCore Ligand. <b>2019</b> , 9, 226		13
1435	A Universal Quantitative Descriptor of the Dispersion Interaction Potential. <b>2019</b> , 58, 9758-9769		23
1434	Exploration of the Luminescence Properties of Organic Phosphate Salts of 3-Quinoline- and 5-Isoquinolineboronic Acid. <b>2019</b> , 2019, 2707-2724		6
1433	Synthesis, crystal structures, spectral FT-IR, NMR and UV-Vis investigations and Hirshfeld surface analysis of two new 2-hydroxyethyl-substituted N-heterocyclic carbene precursors. <b>2019</b> , 66, 1389-1396		6
1432	Synthesis, Crystal Structure and Non-covalent Interactions Analysis of Novel N-substituted Thiosemicarbazone. <b>2019</b> , 35, 471-477		4
1431	Synthesis, crystal structure and Hirshfeld surface analysis of an octa-molybdate, dimethylammonium, (E)-N'-(pyridin-2-ylmethylene)acetohydrazide Co-crystal (1:4:2). <b>2019</b> , 1193, 326-333		0
1430	Evaluation of N-H...O hydrogen bond interactions in two new phosphoric triamides with a P(O)[NHCH(CH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub> segment by means of topological (AIM) calculations, Hirshfeld surface analysis and 3D energy framework approach. <b>2019</b> , 234, 401-413		3
1429	Synthesis, X-ray structure, and DFT studies of five- and eight-coordinated Cd(II) complexes with s-triazine N-pincer chelate. <b>2019</b> , 72, 1621-1636		12
1428	Single-crystal-to-single-crystal guest exchange in columnar assembled brominated triphenylamine bis-urea macrocycles. <i>Chemical Communications</i> , <b>2019</b> , 55, 5619-5622	5.8	16
1427	Seeking the best model for non-covalent interactions within the crystal structure of meloxicam. <b>2019</b> , 1157, 47-53		6
1426	Geometrical Isomerism in Guanabenz Free Base: Synthesis, Characterization, Crystal Structure, and Theoretical Studies. <b>2019</b> , 19, 3183-3191		5

- 1425 Insights into supramolecular assembly formation of diethyl aryl amino methylene malonate (DAM) derivatives assisted via non-covalent interactions. **2019**, 1192, 178-185
- 1424 Synthesis, crystal structure and DFT calculations of a new coumarin-amide binuclear Cu (II) complex. **2019**, 1192, 115-121 4
- 1423 Transfer of chirality in N-triphenylacetyl amino acids and chiral derivatives of N-triphenylacetyl Glycyl dipeptide and control of their assembly with steric constraints. **2019**, 21, 3420-3430 6
- 1422 Crystal structure and Hirshfeld surface analysis of 4-allyl-6-bromo-2-(4-chloro-phen-yl)-4-imidazo[4,5-]pyridine. **2019**, 75, 43-48 1
- 1421 Anomalous pressure dependence of the electronic properties of molecular crystals explained by changes in intermolecular electronic coupling. **2019**, 253, 9-19 1
- 1420 Structure properties of scoparone: Polymorphs and cocrystals. **2019**, 1191, 323-336 6
- 1419 Molecular interaction transfer among solvents and solutes modulates the formation of linezolid crystals. **2019**, 21, 3209-3217 3
- 1418 Experimental and Theoretical Insights into the Optical Properties and Intermolecular Interactions in Push-Pull Bromide Salts. **2019**, 8, 483-496 2
- 1417 Synthesis, X-ray crystal structure and DFT calculations of 2,4-dihydro-10H-spiro [anthracene-9,3'-benzo[b][1,4]thiazin]-10-amine and 1,3,5-triindolyl benzene. **2019**, 21, 100227 2
- 1416 Minor modifications afford improved host selectivities in xanthenyl-type host systems. **2019**, 21, 3000-3013 4
- 1415 Preparation, spectral, structural, thermal and anticancer molecular docking studies of bis-(theophyllinato)-tetraaquocobalt(II) complex. **2019**, 1190, 125-134 3
- 1414 Structure analysis of a phenylpyrazole carboxylic acid derivative crystallizing with three molecules in the asymmetric unit ( $Z' = 3$ ) using X-ray powder diffraction. **2019**, 34, 151-158 2
- 1413 Dibromomanganese(II) complexes with hexamethylphosphoramide and phenylphosphonic bis(diamide) ligands. **2019**, 72, 309-327 15
- 1412 Pressure-Dependent Structural and Luminescence Properties of 1-(Pyren-1-yl)but-2-yn-1-one. **2019**, 24, 4
- 1411 Theoretical Investigations into the Electron and Ambipolar Transport Properties of Anthracene-Based Derivatives. **2019**, 123, 3300-3314 4
- 1410 Synthesis, crystallographic structure, Hirshfeld surface analysis and DFT calculations of two salen-type halogenated Schiff-base Ni(II) complexes. **2019**, 166, 123-129 12
- 1409 Chiral self-assembly of a novel (CuI/ReVII)-heterobimetallic L-Arginine complex: Crystal structure, Hirshfeld surface analysis, spectroscopic properties and biochemical studies. **2019**, 1186, 307-316 3
- 1408 Synthesis, characterization, Hirshfeld surface, cytotoxicity, DNA damage and cell cycle arrest studies of N, N-diphenyl-N'-(biphenyl-4-carbonyl/4-chlorobenzoyl) thiocarbamides. **2019**, 1186, 333-344 7

1407	Structural Arrangement and Computational Exploration of Guanidinium-Based Ionic Liquids with Benzoic Acid Derivatives as Anions. <b>2019</b> , 19, 2642-2657	3
1406	Synthesis and structural DFT studies of Ni(II) and Co(II) complexes with s-triazine-based di-compartmental ligand. <b>2019</b> , 165, 162-170	6
1405	Crystal Structure of a Cationic Bile Salt Derivative ([3,5,7,12]-3-(2-naphthylolamino)-7,12-dihydroxycholan-24-triethylammonium iodide). <b>2019</b> , 9, 135	
1404	High-Spin Mononuclear Iron(III) Complexes with Pentadentate Schiff Base Ligands: Structural Analysis and Magnetic Properties. <b>2019</b> , 84, 358-367	5
1403	Tetranuclear anionic bromobismuthate [Bi4Br18]6- New structural type in halometalate collection. <b>2019</b> , 103, 72-74	6
1402	Molybdenum(VI) complexes of hemilabile aroylhydrazone ligands as efficient catalysts for greener cyclooctene epoxidation: an experimental and theoretical approach. <b>2019</b> , 43, 5531-5542	17
1401	Synthesis, crystal structure, hirshfeld surface analysis, spectroscopic, optical and thermal behavior of new organic-inorganic hybrid material (C7H11N2)2[CrCl2(H2O)4]Cl3·2H2O. <b>2019</b> , 1189, 122-130	2
1400	Synthesis, crystal structure, Hirshfeld surface analysis and DNA binding studies of 1-((E)-3-(4-bromophenyl)-1-phenylallylidene)-2-(m-tolyl)hydrazine. <b>2019</b> , 1189, 112-121	3
1399	Syntheses, Crystal Structures, and Properties of Two Novel CL-20-based Cocrystals. <b>2019</b> , 645, 656-662	9
1398	Synthesis, Crystal Structure, Hirshfeld Surface Analysis, DFT, and DNA-Binding Studies of (E)-2-(3-Hydroxy-4-Methoxybenzylidene)Hydrazinecarbothioamide. <b>2019</b> , 189, 175-192	1
1397	Dicyclohexylammonium O,O'-Diphenyl Phosphate, [(C6H11)2NH2][[(C6H5O)2P(O)(O)]: Spectroscopic Study, Crystal Structure, and Hirshfeld Surface Analysis. <b>2019</b> , 2019, M1051	1
1396	Prediction of the Linear and Nonlinear Optical Properties of a Schiff Base Derivatives via DFT. <b>2019</b> , 2019, 1-12	6
1395	Synthesis, structure, Hirshfeld surface analysis and photophysical studies of red emitting europium acetylacetonate complex incorporating a phenanthroline derivative. <b>2019</b> , 377, 268-281	28
1394	Synthesis, structural characterization, theoretical studies and corrosion inhibition of a new pyrrole derivative: 1-(1-benzyl-4-(4-chlorophenyl)-2,5-dimethyl-1H-pyrrol-3-yl)ethanone. <b>2019</b> , 1189, 240-248	8
1393	Proton-induced intermolecular charge transfer in Picolinium Tartrate Monohydrate crystal for OLED and nonlinear optical applications: A combined experimental and computational study. <b>2019</b> , 165, 239-248	10
1392	Water-Involved Hydrogen Bonds in Dimeric Supramolecular Structures of Magnesium and Zinc Phthalocyaninato Complexes. <b>2019</b> , 4, 3673-3683	3
1391	Redox-cycling and intercalating properties of novel mixed copper(II) complexes with non-steroidal anti-inflammatory drugs tolfenamic, mefenamic and flufenamic acids and phenanthroline functionality: Structure, SOD-mimetic activity, interaction with albumin, DNA damage study and anticancer activity. <b>2019</b> , 194, 97-113	39
1390	Evaluation of structural, optical and mechanical behaviour of L-argininium bis(trifluoroacetate) single crystal: An efficient organic material for second harmonic generation applications. <b>2019</b> , 129, 401-412	6

- 1389 Analysis of two novel 1-4 quinolinone structures with bromine and nitrobenzyl ligands. **2019**, 25, 55 3
- 1388 Synthesis, crystal structure, Hirshfeld Surface analysis, and DFT studies of 16-ferrocenylidene-17 $\beta$ -estra-1,3,5-triene-3,17-diol: Towards the application of ferrocene-hormone conjugates to target hormone dependent breast cancer. **2019**, 1184, 382-388 3
- 1387 Synthesis, crystal structure and 3D energy frameworks of ethyl 2-[5-nitro-2-oxopyridine-1(2H)-yl] acetate: Hirshfeld surface analysis and DFT calculations. **2019**, 20, 100195 9
- 1386 Novel benzofuran based chalcone material for potential nonlinear optical application. **2019**, 560, 191-196 6
- 1385 Synthesis, molecular structure and DFT studies of two heteroleptic nickel(II) s-triazine pincer type complexes. **2019**, 1185, 461-468 8
- 1384 Heterometallic Zn(II)-K(I) complex with salen-type Schiff-base ligand: Synthesis, crystal structure, solid-state photoluminescent property and theoretical study. **2019**, 1185, 112-120 13
- 1383 Gel- and Solid-State-Structure of Dialanine and Diphenylalanine Amphiphiles: Importance of C $\cdots$ H Interactions in Gelation. **2019**, 20, 972-983 11
- 1382 Novel primary amide-based cationic metal complexes: green synthesis, crystal structures, Hirshfeld surface analysis and solvent-free cyanosilylation reaction. **2019**, 48, 3743-3757 4
- 1381 Synthesis and Crystal Structure of Bis(2-phenylpyridine-C,N)-bis(acetonitrile)iridium(III)hexafluorophosphate Showing Three Anion/Cation Couples in the Asymmetric Unit. **2019**, 9, 617 1
- 1380 Two-Dimensional Hydrogen-Bonded Crystal Structure, Hirshfeld Surface Analysis and Morphology Prediction of a New Polymorph of 1H-Nicotinamidium Chloride Salt. **2019**, 9, 571 1
- 1379 Theoretical Insights on the High Pressure Behavior of Pentazolate Anion Complex [Co(HO)(N)] $\cdot$ 4HO. **2019**, 9, 15648 2
- 1378 Crystal structure of ethyl (Z)-(4-oxo-4-phenylbut-2-en-2-yl)glycinate, C<sub>14</sub>H<sub>17</sub>NO<sub>3</sub>. **2019**, 234, 1183-1185 4
- 1377 Formation of a tetranuclear supramolecule via non-covalent Pb $\cdots$ Cl tetrel bonding interaction in a hemidirected lead(II) complex with a nickel(II) containing metaloligand. **2019**, 21, 6859-6868 18
- 1376 Ruthenium(ii) and palladium(ii) homo- and heterobimetallic complexes: synthesis, crystal structures, theoretical calculations and biological studies. **2019**, 48, 15869-15887 4
- 1375 Structural, theoretic and spectroscopic analysis of 2-methyl-5-nitroaniline salts with various inorganic acids. **2019**, 75, 1003-1013 5
- 1374 The first two examples of halogen bonding with a sigma hole-donating fluorine in the C-FO interaction from polyfluorinated trans-dihalo-palladium(ii) di-substituted pyridine complexes. *Chemical Communications*, **2019**, 55, 14259-14262 5.8 12
- 1373 Crystal structure and physical stability of ginsenoside compound-K solvates. **2019**, 21, 7313-7321 2
- 1372 The first coordination polymers with an [O][N]P(S)-Hg segment: a combined experimental, theoretical and database study. **2019**, 48, 17908-17918 1

1371	A Universal Quantitative Descriptor of the Dispersion Interaction Potential. <b>2019</b> , 131, 9860-9871	5
1370	Diethylaminophenyl-based Schiff base Cu(II) and V(IV) complexes: experimental and theoretical studies and cytotoxicity assays. <b>2019</b> , 43, 18832-18842	11
1369	Halogen bonding in the structures of pentaiodobenzoic acid and its salts. <b>2019</b> , 21, 6666-6670	18
1368	Crystal structures, Hirshfeld surface analysis and Pixel energy calculations of three trifluoromethylquinoline derivatives: further analyses of fluorine close contacts in trifluoromethylated derivatives. <b>2019</b> , 74, 791-810	1
1367	Sonication-assisted synthesis of a new rod-like metal-organic coordination polymer compound; novel precursor to produce pure phase nano-sized lead(II) oxide. <b>2019</b> , 1176, 434-446	14
1366	Synthesis, structural characterization, Hirshfeld analyses, and biological activity studies of Ni(II) and Zn(II) complexes containing the sulfonohydrazone group. <b>2019</b> , 484, 87-94	8
1365	Supramolecular association in the triclinic (Z'=1) and monoclinic (Z'=4) polymorphs of 4-(4-acetylphenyl)piperazin-1-ium 2-amino-4-nitrobenzoate. <b>2019</b> , 234, 43-57	18
1364	Co(II), Ni(II) and Cu(II) ternary complexes with sulfadiazine and dimethylformamide: Synthesis, spectroscopic characterization, crystallographic study and antibacterial activity. <b>2019</b> , 1176, 605-613	10
1363	Several salicylatocopper(II) complexes with diethylnicotinamide: Preparation, structure, spectral properties and Hirshfeld surface analysis. <b>2019</b> , 1181, 373-382	5
1362	Spectroscopic, Hirshfeld surface, X-ray diffraction methodologies and local & global chemical activity calculations of 5-(2-methoxy-4-(prop-1-en-1-yl)phenoxy)pyrazine-2,3-dicarbonitrile. <b>2019</b> , 1181, 25-37	25
1361	Effects of Noncovalent Interactions on the Impact Sensitivity of HNS-Based Cocrystals: A DFT Study. <b>2019</b> , 19, 756-767	18
1360	Synthesis, physicochemical and quantum chemical studies on a new organic NLO crystal: Cinnamoylproline. <b>2019</b> , 1180, 826-838	9
1359	A new structural motif for cadmium dithiocarbamates: crystal structures and Hirshfeld surface analyses of homoleptic zinc and cadmium morpholine dithiocarbamates. <b>2019</b> , 234, 341-349	11
1358	Above Room Temperature Spin Transition in Thermally Stable Mononuclear Fe(III) Complexes. <b>2019</b> , 58, 1134-1146	8
1357	Crystal structure, spectroscopic and biological study of a new inorganic-organic hybrid compound [Cd4Cl12(H2O)2]n (C10N4H28)n. <b>2019</b> , 100, 134-143	9
1356	Synthesis, crystal structure, vibrational study, optical properties and Hirshfeld surface analysis of bis(2,6-diaminopyridinium) tetrachloridocobaltate(II) monohydrate. <b>2019</b> , 1180, 72-80	18
1355	Experimental and theoretical investigations of the molecular structure, the spectroscopic properties and TD-DFT analysis of a new semiconductor hybrid based iron(III). <b>2019</b> , 23, 600-611	3
1354	Characterization and properties of a new energetic co-crystal composed of trinitrotoluene and 2,6-diaminotoluene. <b>2019</b> , 1179, 453-461	10

1353	Deciphering the Multifarious Charge-Transport Behaviour of Crystalline Propeller-Shaped Triphenylamine Analogues. <b>2019</b> , 25, 1992-2002	9
1352	Supramolecular diversity in solid-state architecture formed between the 1-(diaminomethylene)thiourea and citric acid. <b>2019</b> , 1182, 9-21	9
1351	A new non-centrosymmetric Chlorobismuthate(III) hybrid material: Crystal structure, optical properties and antibacterial study. <b>2019</b> , 1181, 338-347	12
1350	A hybrid perchlorate with a low band gap: Crystal structure, physicochemical characterization and Hirshfeld surfaces study. <b>2019</b> , 1181, 300-304	5
1349	2,5-Furandicarboxylic acid as a linker for lanthanide coordination polymers: the role of heteroaromatic $\pi$ -stacking and hydrogen bonding. <b>2019</b> , 43, 2179-2195	25
1348	Self-assembly and supramolecular isomerism in copper (II) coordination compounds of pyridine-4-carboxamide based ligand. <b>2019</b> , 486, 74-82	3
1347	On the influence of small chemical changes upon the supramolecular association in substituted 2-(phenoxy)-1,4-naphthoquinones. <b>2019</b> , 234, 183-200	1
1346	Homochiral Asymmetric-Shaped Electron-Transporting Materials for Efficient Non-Fullerene Perovskite Solar Cells. <b>2019</b> , 12, 224-230	24
1345	The first isolated Manganese(II) porphyrin N-Heterocyclic carbenes: Synthesis and spectroscopic characterizations. <b>2019</b> , 162, 75-79	6
1344	Synthesis, Elucidation, Hirshfeld surface analysis, and DFT calculations of 4-chloro-N-[2-(2-1H-indol-3-yl-acetylamino)-phenyl]-benzamide. <b>2019</b> , 1178, 384-393	20
1343	Steric control of supramolecular association in structures of Zn(S2COR)2 with N,N'-bis(pyridin-4-ylmethyl)oxalamide. <b>2019</b> , 234, 165-175	6
1342	Two nitrates of dapsone: New candidates for non-linear optical materials. <b>2019</b> , 1178, 375-383	4
1341	Synthesis, spectroscopic properties, crystal structure, antimicrobial properties and molecular docking studies of the complex (1) 3(C36H24MnN6)·6(PF6). 0.5H2O. <b>2019</b> , 1180, 438-446	2
1340	Metal-Involving Bifurcated Halogen Bonding $\text{CBr}^{\delta-}\cdots\text{I}^{\delta+}(\text{ClPt})$ . <b>2019</b> , 19, 1364-1376	33
1339	A Practical Guide to the Design of Molecular Crystals. <b>2019</b> , 19, 1426-1453	143
1338	Spectroscopic identification, structural features, Hirshfeld surface analysis and molecular docking studies on stiripentol: An orphan antiepileptic drug. <b>2019</b> , 1180, 110-118	5
1337	2-thioxo-3N-(2-methoxyphenyl) $\pi$ [4?-methyl -3?N -(2?-methoxyphenyl) thiazol-2?(3?H)-ylidene] thiazolidin-4-one: Synthesis, characterization, X-ray single crystal structure investigation and quantum chemical calculations. <b>2019</b> , 1177, 186-192	8
1336	Phase transition in polar 2-nitroanilinium nitrate. Graph-set approach of hydrogen bonding patterns and analysis of vibrational spectra. <b>2019</b> , 207, 313-320	4

1335	Discovery of new potential triplet acting inhibitor for Alzheimer's disease via X-ray crystallography, molecular docking and molecular dynamics. <b>2020</b> , 38, 1903-1917	5
1334	Synthesis, crystal structure and intermolecular contacts in trans-bis(ethylamine) dichloro platinum(II) and palladium(II) complexes. <b>2020</b> , 1199, 126983	
1333	A copper(II) zig-zag metalorganic coordination polymer: synthesis, crystal structure, topology study, hirshfeld surface analysis and survey different conditions on morphology of a novel nano structure [Cu(L)(SCN)(H <sub>2</sub> O) <sub>2</sub> ] <sub>n</sub> .2H <sub>2</sub> O. <b>2020</b> , 50, 80-93	3
1332	Synthesis, characterization and hydrogen bonding attributes of halogen bonded O-hydroxy Schiff bases: Crystal structure, Hirshfeld surface analysis and DFT studies. <b>2020</b> , 1202, 127238	6
1331	A rare flattened tetrahedral Mn(II) salen type complex: Synthesis, crystal structure, biomimetic catalysis and DFT study. <b>2020</b> , 499, 119176	9
1330	Synthesis, Photophysical and Electronic Properties of New Red-to-NIR Emitting Donor-Acceptor Pyrene Derivatives. <b>2020</b> , 26, 438-453	17
1329	Zn(II) complex derived from bidentate Schiff base ligand: Synthesis, characterization, DFT studies and evaluation of anti-inflammatory activity. <b>2020</b> , 1201, 127177	10
1328	Assessing the impact on aqueous solubility of berberine chloride via co-crystallization with different stoichiometric ratios of pyromellitic dianhydride. <b>2020</b> , 1200, 127086	7
1327	Ethanol coordinated zinc trimethoxyphenylporphyrin: Structure, theoretical studies and formation of isoporphyrin. <b>2020</b> , 1200, 127116	4
1326	Synthesis and characterization of a double oximate bridged dimeric copper(II) complex and its use in oxidative dimerisation of o-aminophenol. <b>2020</b> , 175, 114164	12
1325	Design-based synthesis, molecular docking analysis of an anti-inflammatory drug, and geometrical optimization and interaction energy studies of an indole acetamide derivative. <b>2020</b> , 1202, 127244	16
1324	Synthesis, spectral characterization (FT-IR, NMR, XRD) and computational studies of chloroacetyl chloride incorporated 3t-butyl-2r,6c-diphenyl/di(thiophen-2-yl)piperidin-4-ones. <b>2020</b> , 1200, 127076	2
1323	Synthesis, structure, in silico ADME evaluation and in vitro antioxidant of (E)-N-(4-ethylphenyl)-2-(isomeric methylbenzylidene)thiosemicarbazone derivatives. <b>2020</b> , 1199, 126972	2
1322	Structural, spectroscopic and theoretical studies of sodium (2-carbamoylphenoxy) acetate salt. <b>2020</b> , 1200, 127016	1
1321	Formation of supramolecular hydrogen-bonding chains and networks from copper (II) halogenobenzoates with N-methylnicotinamide: Supramolecular isomerism. <b>2020</b> , 175, 114237	1
1320	Synthesis, characterisation, Hirshfeld surface and in vitro cytotoxicity evaluation of new N-aryl-N'-Alkoxy carbonyl thiocarbamide derivatives. <b>2020</b> , 1202, 127269	2
1319	The crystal structure and solution behaviour of decyl- and dodecyl $\beta$ -D-lyxopyranoside: X-ray, NMR, computational and Hirshfeld surface analysis. <b>2020</b> , 1202, 127348	2
1318	Synthesis, computational studies and biological activity of oxamohydrazide derivatives bearing isatin and ferrocene scaffolds. <b>2020</b> , 1202, 127372	2

- 1317 The role of weak interactions in the crystal packing of two novel 1D Hg(II) coordination polymers and investigation for preparation of their rod and spherical structures. **2020**, 501, 119243 1
- 1316 Cu(II) and Zn(II) complexes from a thiosemicarbazone derivative: Investigating the intermolecular interactions, crystal structures and cytotoxicity. **2020**, 1202, 127319 6
- 1315 Comparative X-ray, vibrational, theoretical and biological studies of new in situ formed [CoLSX]<sub>2</sub>[CdX<sub>4</sub>] halogenocadmate(II) complexes containing N-scorpionate ligand. **2020**, 175, 114229 2
- 1314 Syntheses, spectroscopy, tautomerism, induced chirality and molecular structure of 3-(o/p-tolylimino)indolin-2-one and bis[3-(o/p-tolylimino)indole-2-olato- $\lambda$ N,O]-Zinc(II). **2020**, 501, 119245 3
- 1313 Single-ion magnet behavior of two pentacoordinate Co(II) complexes with a pincer ligand 2,6-bis(imidazo[1,5-a]pyridin-3-yl)pyridine. **2020**, 31, 547-555 3
- 1312 Intermolecular forces regulated the dimensions of Co(II), Cu(II) complexes with 2-(1H-1,2,4-Triazol-3-yl)pyridine. **2020**, 111, 107613 1
- 1311 Analysis of hydrogen bonding and weak interactions in the crystal structure of (E)-N-(4-ethylphenyl)-2-(4-hydroxybenzylidene)thiosemicarbazone: experimental and theoretical studies. **2020**, 118, e1670878
- 1310 Crystal Structure at the Origin of the Thermal Stability and Large Enthalpy of Fusion and Sublimation Values of Calixarenes. **2020**, 20, 1302-1310 3
- 1309 A Cu(II)-Inorganic Co(II) Crystal as a Versatile Catalyst Towards Click Chemistry for Synthesis of 1,2,3-triazoles and  $\alpha$ -hydroxy-1,2,3-triazoles. **2020**, 5, 75-82 16
- 1308 Two-dimensional halogen-bonded organic frameworks based on the tetrabromobenzene-1,4-dicarboxylic acid building molecule. **2020**, 22, 24-34 8
- 1307 Crystal structure evolution of the high energetic compound carbonic dihydrazidinium bis[3-(5-nitroimino-1,2,4-triazolate)] induced by solvents. **2020**, 22, 593-601 3
- 1306 Exploring the semiconductor properties of a charge transfer cocrystal of 1-aminopyrene and TCNQ. **2020**, 22, 720-727 10
- 1305 Hexaiododiplatinate(II) as a useful supramolecular synthon for halogen bond involving crystal engineering. **2020**, 49, 356-367 20
- 1304 Synthesis, spectral, thermal, structural, optical characterization, and Hirshfeld surface analysis of N,N-diethylnicotinamide complexes of Mn(II) and Co(II) 4-cyanobenzoates. **2020**, 74, 2021-2033
- 1303 Modulation of Weak Interactions in Structural Isomers: Positional Isomeric Effects on Crystal Packing and Physical Properties and Solid-State Thin-Film Fabrication. **2020**, 5, 448-459 11
- 1302 Metal-involving halogen bond Ar<sup>+</sup>[dz<sub>2</sub>Pt(II)] in a platinum acetylacetonate complex. **2020**, 22, 554-563 20
- 1301 A one-pot route to N-acyl ureas: a formal four-component hydrolytic reaction involving aminonitrones and isocyanide dibromides. **2020**, 44, 1253-1262 5
- 1300 Synthesis of a novel phenytoin derivative: Crystal structure, Hirshfeld surface analysis and DFT calculations. **2020**, 1205, 127630 22



1299	Synthesis, crystal structure, Hirshfeld surface analysis and DFT calculations of 2-[(2,3-dimethylphenyl)amino]-N[(E)-thiophen-2-ylmethylidene]benzohydrazide. <b>2020</b> , 1205, 127654	23
1298	Experimental and DFT/TD-DFT approach on photo-physical and NLO properties of 2, 6-bis (4-Chlorobenzylidene) cyclohexanone. <b>2020</b> , 100, 109620	1
1297	Systematical Investigation of Chain Length Effect on the Melting Point of a Series of Bifunctional Anthraquinone Derivatives via X-ray Diffraction and Scanning Tunneling Microscopy. <b>2020</b> , 124, 1646-1654	7
1296	Molecular and Crystal Features of Thermostable Energetic Materials: Guidelines for Architecture of "Bridged" Compounds. <b>2020</b> , 6, 54-75	49
1295	Synthesis, characterisation and energetic performance of insensitive energetic salts formed between picric acid and 2,3-diaminotoluene, 2,4-diaminotoluene. <b>2020</b> , 1205, 127580	5
1294	Host Polytypism and Structural Modulation in Two-Dimensional Fe(NCS) <sub>2</sub> -Based Metal-Organic Frameworks: Can Spin-Crossover Transitions Be Predicted?. <b>2020</b> , 20, 422-433	1
1293	Synthesis and structural characterization of a series of ternary copper(II)-L-dipeptide-neocuproine complexes. Study of their cytotoxicity against cancer cells including MDA-MB-231, triple negative breast cancer cells. <b>2020</b> , 203, 110930	11
1292	Possible pre-phase transition of the $\beta$ -HMX crystal observed by the variation of hydrogen-bonding network under high pressures. <b>2020</b> , 22, 330-348	4
1291	Unraveling the unusual effect of fluorination on crystal packing in an organic semiconductor. <b>2020</b> , 22, 1665-1673	9
1290	Intermolecular Interactions and Intramolecular Couplings of Binuclear Porphyrin Models for Cytochrome Oxidase. <b>2020</b> , 59, 1242-1255	1
1289	Coordination properties of diethylenetriamine in relation to zinc phthalocyanine. <b>2020</b> , 178, 114313	5
1288	Reverse Sandwich Structures from Interplay between Lone Pair-Hole Atom-Directed C <sup>≡</sup> N <sub>2</sub> [M] and Halogen Bond Interactions. <b>2020</b> , 20, 995-1008	21
1287	Synthesis, structure elucidation and surface analysis of a new single crystal N-((2-(benzo [4,5]imidazo [1,2-c]quinazolin-6-yl)phenyl)carbamothioyl)heptanamide: Theoretical and experimental DNA binding studies. <b>2020</b> , 1205, 127496	7
1286	Heteroleptic copper(II) complexes with 2-bromo-5-methylpyridine: Structures, features of non-covalent interactions and magnetic behavior. <b>2020</b> , 502, 119333	1
1285	Understanding the Formation of Novel Hydrated Gallic Acid-Creatinine Molecular Salt: Crystal Structure, Hirshfeld Surface and DFT Studies. <b>2020</b> , 50, 410-421	2
1284	Physico-chemical characterization and computational studies of a new organic adduct 3-amino-2-chloropyridine: Benzilic acid, crystal for third order harmonic generation. <b>2020</b> , 1203, 127415	5
1283	Crystal structure, Hirshfeld surface analysis and physicochemical studies of two new Cu(II) complexes with the ligand 2-amino-6-methylpyrimidin-4-(1H)-one. <b>2020</b> , 502, 119289	
1282	Mononuclear and binuclear dioxidomolybdenum(VI) complexes of ONO appended aroylhydrazone: Crystal structures, interaction energy calculation and cytotoxicity. <b>2020</b> , 1204, 127467	6

1281	Experimental and theoretical approach: Local and global chemical activity, charge transfer method with DNA bases, spectroscopic, structural and electronic properties of (E)-2-(((4-fluorophenyl)imino)methyl)-4-methoxyphenol. <b>2020</b> , 1204, 127451	6
1280	Exploring the highly dense energetic materials via regiochemical modulation: A comparative study of two fluorodinitromethyl-functionalized herringbone trifuroxans. <b>2020</b> , 391, 123573	16
1279	Quantitative investigation on the intermolecular interactions present in 8-(4-ethoxyphenyl)-1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione with insight from interaction energies, energy framework, electrostatic potential map and fingerprint analysis. <b>2020</b> , 132, 1	3
1278	Cocrystallization of 2,4-Diamino-6-phenyl-1,3,5-triazine with $\pi$ (phenylthio)propionic acid: Crystal structure, Hirshfeld surface, DFT studies and molecular docking. <b>2020</b> , 29, 100520	
1277	Structure and surface analysis of ibuprofen-organotin conjugate: Potential anti-cancer drug candidacy of the compound is proven by in-vitro DNA binding and cytotoxicity studies. <b>2020</b> , 192, 114845	3
1276	The significant role of molecular dipole arrangements on the second and third-order nonlinear optical properties of a furan based chalcone. <b>2020</b> , 599, 412501	2
1275	Synthesis, Crystal and DFT studies of Zn/Co complexes of Dehydroacetic acid using ligand exchange approach. <b>2020</b> , 122, 108280	2
1274	Design and synthesis of coumarin-triazole hybrids: biocompatible anti-diabetic agents, molecular docking and ADME screening. <b>2020</b> , 6, e05290	6
1273	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. <b>2020</b> , 44, 19541-19554	10
1272	A one-dimensional switchable dielectric material with Pd uptake function: [(CH)NHS]BiCl. <i>Chemical Communications</i> , <b>2020</b> , 56, 13764-13767	5.8 7
1271	Novel nitro based chalcone derivative single crystals: characterization on structural, linear optical, thermal, and third-order nonlinear optical properties. <b>2020</b> , 126, 1	2
1270	Synthesis, characterization, and crystal structure analysis of group IIB coordination compounds containing N,N'-bidentate chelating Schiff-base ligand. <b>2020</b> , 73, 3044-3061	
1269	Synthesis of 5-(1H-pyrazol-1-yl)-2H-tetrazole-derived energetic salts with high thermal stability and low sensitivity. <b>2020</b> , 1, 83-89	6
1268	Synthesis, structural characterization, Hirshfeld surface and DFT based reactivity, UV filter and NLO studies of Schiff base analogue of 4-aminoantipyrine. <b>2020</b> , 2, 100062	4
1267	A highly stable octa-coordinated energetic complex. <b>2020</b> , 22, 6591-6595	0
1266	Hirshfeld Surface Analysis and Fingerprint Plots in Determining the Resemblance of a New Copper Coordination Polymer Synthesized by Two Different Methods. <b>2020</b> , 61, 274-282	
1265	Hg(II) coordination compounds containing tridentate NNO Schiff-base ligand: synthesis, characterization, and crystal structure analysis. <b>2020</b> , 151, 1077-1085	
1264	Crystal Structure and Hirshfeld Surface Analysis of 3,5-Bis(4-Methoxyphenyl)-4,5-Dihydro-1H-Pyrazole-1-Carbothioamide. <b>2020</b> , 61, 126-132	3

1263	Bimetallic and trimetallic Cd(II) and Hg(II) mixed-ligand complexes with 1,1-dicyanoethylene-2,2-dithiolate and polyamines: Synthesis, crystal structure, Hirshfeld surface analysis, and antimicrobial study. <b>2020</b> , 512, 119877	14
1262	Crystal structure, Hirshfeld surface analysis, thermal and DFT investigation accomplished with photoluminescence study of bis(N, N-diethylethylenediammonium)decabromodiantimoinate(III). <b>2020</b> , 1221, 128828	1
1261	Experimental and theoretical studies of 2-Mercaptobenzothiazole with 2-Bromomethylmesitylene and 1,4-Bis(bromomethyl)durene. <b>2020</b> , 1222, 128894	4
1260	Imine-Benzoic Acid Cocrystals as a Tool to Study Intermolecular Interactions in Schiff Bases. <b>2020</b> , 20, 2240-2250	9
1259	Highly selective sensing of Fe/Hg and proton conduction using two fluorescent Zn(ii) coordination polymers. <b>2020</b> , 49, 11129-11141	15
1258	Structure, Antimicrobial Activity, Hirshfeld Analysis, and Docking Studies of Three Silver(I) Complexes-Based Pyridine Ligands. <b>2020</b> , 10, 4853	1
1257	Supramolecular interactions in a family of dinuclear helicites in the solid-state. <b>2020</b> , 32, 456-465	
1256	Halogen bonding between entirely negative fluorine atoms? Evidence from the crystal packing of some gold(I) and gold(III) complexes with extensively fluorinated m-terphenyl ligands and triphenylphosphane. <b>2020</b> , 22, 8285-8289	1
1255	Chemistry of transition-metal complexes containing functionalized phosphines: synthesis and structural analysis of rhodium(I) complexes containing allyl and cyanoalkylphosphines. <b>2020</b> , 76, 932-946	
1254	Crystal Engineering of Molecular Solids as Temporary Adhesives. <b>2020</b> , 32, 9882-9896	7
1253	Crystal Structure and Hirshfeld Surface Analysis of (E)-1-(4-Bromophenyl)-2-(2,2-Dichloro-1-(4-Fluorophenyl)vinyl)diazene. <b>2020</b> , 65, 1169-1172	2
1252	The supramolecular self-assembly of 5-fluorouracil and caffeic acid through cocrystallization strategy opens up a new way for the development of synergistic antitumor pharmaceutical cocrystal. <b>2020</b> , 22, 7992-8006	4
1251	Quantitative Investigation of Weak Intermolecular Interactions of $\beta$ and $\alpha$ F3 Substituted in Situ Cryocrystallized Benzaldehydes. <b>2020</b> , 20, 7921-7933	3
1250	Enabling Control over Mechanical Conformity and Luminescence in Molecular Crystals: Interaction Engineering in Action. <b>2020</b> , 26, 14488-14495	3
1249	Crystal structure, hydrogen bonding interactions, Hirshfeld surface analysis and DFT Studies of 4,4'-dicarboxy-2,2'-bipyridinium chloride. <b>2020</b> , 29, 100502	1
1248	New salicylaldehyde azine esters: Structural, aggregation induced fluorescence, electrochemical and theoretical studies. <b>2020</b> , 318, 114029	1
1247	On the Rationalization of Formation of Solvates: Experimental and Computational Study of Solid Forms of Several Nitrobenzoic Acid Derivatives. <b>2020</b> , 20, 5767-5784	6
1246	Quasi-Isostructural Co(II) and Ni(II) Complexes with Mefenamato Ligand: Synthesis, Characterization, and Biological Activity. <b>2020</b> , 25,	4

1245	Recurrent $\pi$ -stacking motifs in three new 4,5-dihydropyrazolyl-1,2,4-triazole-coumarin hybrids: X-ray characterization, Hirshfeld surface analysis and DFT calculations. <b>2020</b> , 44, 14592-14603	28
1244	A new homobimetallic cobalt(II) complex based on the tetradentate 3,5-bis(2-pyridyl)-1H-1,2,4-triazole ligand: Synthesis, crystal structure, Hirshfeld analysis, spectroscopic characterization, magnetic properties and antimicrobial activities. <b>2020</b> , 189, 114722	3
1243	Molecular Engineering of Hexaazatriphenylene Derivatives toward More Efficient Electron-Transporting Materials for Inverted Perovskite Solar Cells. <b>2020</b> , 12, 38222-38231	13
1242	Structural Elucidation of the Mechanism of Molecular Recognition in Chiral Crystalline Sponges. <b>2020</b> , 132, 17753-17759	8
1241	Elucidating the Polymorphic Behavior of Curcumin during Antisolvent Crystallization: Insights from Raman Spectroscopy and Molecular Modeling. <b>2020</b> , 20, 6008-6023	6
1240	Novel one-dimensional polymeric Cu(II) complexes via Cu(II)-assisted hydrolysis of the 2,4-bis(3,5-dimethyl-1H-pyrazol-1-yl)-6-methoxy-1,3,5-triazine pincer ligand: Synthesis, structure, and antimicrobial activities. <b>2020</b> , 34, e5941	6
1239	Crystallization Induced Enhanced Emission in Two New Zn(II) and Cd(II) Supramolecular Coordination Complexes with the 1-(3,4-Dimethylphenyl)-5-Methyl-1,2,3-Triazole-4-Carboxylate Ligand. <b>2020</b> , 12,	5
1238	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. <b>2020</b> , 44, 15515-15525	2
1237	Understanding the structural properties of p-xylylenebis(triphenylphosphonium) cation under different pH and anion conditions. <b>2020</b> , 22, 7704-7715	0
1236	Synthesis, X-ray characterization and theoretical study of 3a,6:7,9a-diepoxybenzo[de]isoquinoline derivatives: on the importance of F $\cdots$ O interactions. <b>2020</b> , 44, 20167-20180	6
1235	Divalent zinc complex of succinylsulfathiazole: Synthesis, spectral, molecular structure, DNA interaction profile and Hirshfeld surface analysis. <b>2020</b> , 122, 108318	0
1234	Synthesis, X-ray Structure, Hirshfeld Analysis of Biologically Active Mn(II) Pincer Complexes Based on s-Triazine Ligands. <b>2020</b> , 10, 931	2
1233	Crystal Engineering Construction of Caffeic Acid Derivatives with Potential Applications in Pharmaceuticals and Degradable Polymeric Materials. <b>2020</b> , 22, 7847-7857	1
1232	On the supramolecular properties of neutral, anionic and cationic cadmium complexes harvested from dithiolate-polyamine binary ligand systems. <b>2020</b> , 22, 8023-8035	3
1231	N-(2,3,5,6-Tetrafluoropyridyl)sulfoximines: synthesis, X-ray crystallography, and halogen bonding. <b>2020</b> , 7, 3896-3906	4
1230	Synthesis, characterization, X-ray structure, electrochemistry, photocatalytic activity and DFT studies of heterotrinnuclear Ni(II), Pd(II) and Zn(II) complexes containing a formylferrocene thiosemicarbazone ligand. <b>2020</b> , 34, e5974	1
1229	Turn-on solid state luminescence by solvent-induced modification of intermolecular interactions. <b>2020</b> , 8, 15742-15750	4
1228	Green Synthesis, SC-XRD, Non-Covalent Interactive Potential and Electronic Communication via DFT Exploration of Pyridine-Based Hydrazone. <b>2020</b> , 10, 778	11

- 1227 Quantitative analysis of intermolecular interactions in cocrystals and a pair of polymorphous cocrystal hydrates from 1,4-dihydroquinoxaline-2,3-dione and 1H-benzo[d]imidazol-2(3H)-one with 2,5-dihydroxy-1,4-benzoquinones: a combined X-ray structural and theoretical analysis. **2020**, 22, 6645-6660 2
- 1226 Hydrogen bonding interactions in fluorinated 1,2,3-triazole derivatives. **2020**, 44, 16006-16019 2
- 1225 Modulation of the Structure and Photoluminescence of Bismuth(III) Chloride Hybrids by Altering the Ionic-Liquid Cations. **2020**, 59, 13465-13472 12
- 1224 Steric Effect of a Capping Ligand on the Formation of Supramolecular Coordination Networks of Ni(II): Solid-State Entrapment of Cyclic Water Dimer. **2020**, 5, 21873-21882 1
- 1223 Cyclic hexapeptoids with N-alkyl side chains: solid-state assembly and thermal behaviour. **2020**, 22, 6371-6384 3
- 1222 Anomalous Melting Point of Multicharge Ionic Liquids: Structural, Electrostatic, and Orbital Properties of [Ln(NO)] (Ln = Ce, Pr) Anions. **2020**, 59, 13700-13708 1
- 1221 Recurrent motifs in pharmaceutical cocrystals involving glycolic acid: X-ray characterization, Hirshfeld surface analysis and DFT calculations. **2020**, 22, 6674-6689 10
- 1220 Transition Metal Complexes with Flufenamic Acid for Pharmaceutical Applications-A Novel Three-Centered Coordination Polymer of Mn(II) Flufenamate. **2020**, 13, 2
- 1219 Rapid Sequentially Palladium Catalyzed Four-Component Synthesis of Novel Fluorescent Biaryl-Substituted Isoxazoles. **2020**, 10, 1412 1
- 1218 Fe(III) Complexes Based on Mono and Bis-pyrazolyl-triazine Ligands: Synthesis, Molecular Structure, Hirshfeld, and Antimicrobial Evaluations. **2020**, 25, 4
- 1217 Synthesis and characterization of zinc(II) complexes with new pyridine-based ligands: crystal structure, Hirshfeld surface analysis, and molecular docking study of lung cancer cell. **2020**, 73, 3203-3222 3
- 1216 A system dynamic of the harvesting strategies to sustain the population of squid using logistic growth model. **2020**, 1613, 012072
- 1215 Single Crystal X-Ray Structure for the Disordered Two Independent Molecules of Novel Isoflavone: Synthesis, Hirshfeld Surface Analysis, Inhibition and Docking Studies on IKK $\beta$  3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-6,7-dimethoxy-4H-chromen-4-one. **2020**, 10, 911 1
- 1214 Halogenated Diazabutadiene Dyes: Synthesis, Structures, Supramolecular Features, and Theoretical Studies. **2020**, 25, 16
- 1213 Synthesis, experimental and in silico studies of N-fluorenylmethoxycarbonyl-O-tert-butyl-N-methyltyrosine, coupled with CSD data: a survey of interactions in the crystal structures of Fmoc-amino acids. **2020**, 76, 328-345 5
- 1212 1D and 2D Silver-Based Coordination Polymers with Thiomorpholine-4-carbonitrile and Aromatic Polyoxoacids as Coligands: Structure, Photocatalysis, Photoluminescence, and TD-DFT Study. **2020**, 20, 4461-4478 5
- 1211 Architecting layered molecular packing in substituted benzobisbenzothiophene (BBBT) semiconductor crystals. **2020**, 22, 3618-3626 8
- 1210 Tetrachloroplatinate(II) anion as a square-planar tecton for crystal engineering involving halogen bonding. **2020**, 22, 4180-4189 8

- 1209 Recognition-Control and Host-Guest Interactions in High-Symmetry Cocrystals of Fullerenes with Cubane and Mesitylene. **2020**, 20, 4169-4175 0
- 1208 Linking triptycene to silole: a fruitful association. **2020**, 4, 2006-2017 2
- 1207 Structural, Hirshfeld surface and in vitro cytotoxicity evaluation of five new N-aryl-N-alkoxycarbonyl thiocarbamide derivatives. **2020**, 195, 812-820
- 1206 Crystal structure, physical study and Hirshfeld surface analysis of (C<sub>9</sub>H<sub>26</sub>N<sub>4</sub>)[SnCl<sub>6</sub>]Cl<sub>2</sub>·2H<sub>2</sub>O. **2020**, 118, 107981
- 1205 Structure: function relationships for thermal and light-induced spin-crossover in isomorphous molecular materials. **2020**, 8, 8420-8429 9
- 1204 Red-emitting CaSc<sub>2</sub>O<sub>4</sub>:Eu<sup>3+</sup> phosphor for NUV-based warm white LEDs: structural elucidation and Hirshfeld surface analysis. **2020**, 44, 8328-8339 15
- 1203 Hydrogen bonding supramolecular networks of copper(II) 2-chronicotinate complexes with picolinamide, nicotinamide, N-methyl-nicotinamide, 2-pyridylmethanol and 4-pyridylmethanol: Hirshfeld surface analysis and spectral properties. **2020**, 74, 3727-3740
- 1202 Crystal Structure and Hirshfeld Surface Analysis of Acetoacetanilide Based Reaction Products. **2020**, 25, 14
- 1201 Syntheses, structure, Hirshfeld analysis and antimicrobial activity of four new Co(II) complexes with s-triazine-based pincer ligand. **2020**, 510, 119753 11
- 1200 Characterization, Hirshfeld surface analysis and vibrational properties of 2,6-diaminopurinium chloride tetrachloroantimonates(III) monohydrate (C<sub>5</sub>H<sub>8</sub>N<sub>6</sub>)[SbCl<sub>4</sub>]Cl·H<sub>2</sub>O. **2020**, 1217, 128386 5
- 1199 Physical characterizations, Hirshfeld surface analysis and luminescent properties of Cd(II) and Pb(II) coordination polymers based on 3-(1,2,4-triazol-1-yl)-benzoic acid. **2020**, 508, 119657 1
- 1198 Synthesis, spectral, structural and antibacterial studies of ONO donor aroylhydrazone and its Mo(VI) complex. **2020**, 1213, 128188 3
- 1197 Synthesis, experimental and theoretical characterization of (E)-2-((2,3-dimethylphenyl)amino)-N-(furan-2-ylmethylene)benzohydrazide. **2020**, 1219, 128518 2
- 1196 Novel 1-D copper(II) coordination polymer based on 2,5-bis(pyridine-2-yl)-1,3,4-thiadiazole as bridging ligand: Synthesis, crystal structure, Hirshfeld surface analysis, spectroscopic characterizations and biological assessment. **2020**, 1218, 128533 6
- 1195 Morphotropism and Quasi-Isostructurality in the Three High Z? Concomitant Polymorphs of Efinaconazole. **2020**, 20, 4238-4242 5
- 1194 Synthesis, structural insights and catalytic activity of a dioxidomolybdenum(VI) complex chelated with N4-(3-methoxyphenyl) thiosemicarbazone. **2020**, 45, 467-476 4
- 1193 Structural, Hirshfeld Surface Analysis, Morphological Approach, and Spectroscopic Study of New Hybrid Iodobismuthate Containing Tetranuclear OD Cluster Bi<sub>4</sub>I<sub>16</sub>·4(C<sub>6</sub>H<sub>9</sub>N<sub>2</sub>)·2(H<sub>2</sub>O). **2020**, 10, 397 7
- 1192 An insight into the potent antioxidant activity of a dithiocarbohydrazone appended cis-dioxidomolybdenum (VI) complexes. **2020**, 34, e5762 3

1191	Synthesis, structure and in vitro anticancer activity of Pd(II) complexes of mono- and bis-pyrazolyl-s-triazine ligands. <b>2020</b> , 187, 114665	2
1190	Effects of Temperature and Solvent Properties on the Liquid-Solid Phase Equilibrium of Pyrazinamide. <b>2020</b> , 65, 3667-3678	5
1189	The Soft Molecular Polycrystalline Ferroelectric Realized by the Fluorination Effect. <b>2020</b> , 142, 12486-12492	41
1188	Crystal Structure and Hirshfeld Surface Analysis of Bis(Triethanolamine)Nickel(II) Dinitrate Complex and a Revelation of Its Characteristics via Spectroscopic, Electrochemical and DFT Studies Towards a Promising Precursor for Metal Oxides Synthesis. <b>2020</b> , 10, 474	2
1187	Persistent Room Temperature Phosphorescence from Triarylboranes: A Combined Experimental and Theoretical Study. <b>2020</b> , 132, 17285-17292	6
1186	Persistent Room Temperature Phosphorescence from Triarylboranes: A Combined Experimental and Theoretical Study. <b>2020</b> , 59, 17137-17144	34
1185	A Hirshfeld surface analysis, crystal structure and infrared characterization of rubidium selenate. <b>2020</b> , 28, 100463	2
1184	Response of Hirshfeld Surface to Structural Modifications in Transition-Metal Coordination Compounds. <b>2020</b> , 20, 4827-4838	4
1183	Synthesis of Cyclometalated Platinum(II) Complex with an Alkynyl-Substituted Isocyanide Ligand, Its Structure and Photophysical Properties. <b>2020</b> , 90, 648-654	3
1182	Evaluation of charge assisted hydrogen bonds in L-(S)-lysinium L-(S)-mandelate dihydrate and L-(S)-alanine L-(S)-mandelic acid complexes: Inputs from Hirshfeld surface, PIXEL energy and QTAIM analysis. <b>2020</b> , 1220, 128701	2
1181	Synthesis, crystal structure, hirshfeld surface analysis, DFT computations and molecular dynamics study of 2-(benzyloxy)-3-phenylquinoxaline. <b>2020</b> , 1221, 128727	6
1180	Novel copper(II) complexes with fenamates and isonicotinamide: structure and properties, and interactions with DNA and serum albumin. <b>2020</b> , 44, 12827-12842	9
1179	Role of Imidazole Co-ligand in the Supramolecular Network of a Co(II) Complex with Sulfadiazine: Crystal Structure, Hirshfeld Surface Analysis and Energetic Calculations. <b>2020</b> , 5, 6331-6338	7
1178	Synthesis and characterization of a new class of phenothiazine molecules with 10H-substituted morpholine & piperidine derivatives: A structural insight. <b>2020</b> , 1219, 128546	4
1177	Molecular and supramolecular structures of self-assembled Cu(II) and Co(II) complexes with 4,4-[6-(3,5-dimethyl-1H-pyrazol-1-yl)-1,3,5-triazine-2,4-diyl]dimorpholine ligand. <b>2020</b> , 1219, 128584	0
1176	1,2,4-triazole-3-thione Schiff bases compounds: Crystal structure, hirshfeld surface analysis, DFT studies and biological evaluation. <b>2020</b> , 1219, 128591	6
1175	Effect of anions on the solid-state interplay of symmetric and unsymmetric phosphonium cations. <b>2020</b> , 44, 10220-10228	2
1174	Lasing Properties Activation by Constitutional Isomerism of an Electron-Accepting Group. <b>2020</b> , 124, 13845-13857	

1173	Synthesis and structural studies on ()-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one: a promising nonlinear optical material.. <b>2020</b> , 10, 22542-22555	6
1172	One-Pot Route to X-perfluoroarenes (X = Br, I) Based on FeIII-Assisted C <sup>6</sup> Functionalization and Utilization of These Arenes as Building Blocks for Crystal Engineering Involving Halogen Bonding. <b>2020</b> , 20, 5908-5921	26
1171	A Series of Manganese(III) Salen Complexes as a Result of Team-Based Inquiry in a Transnational Education Programme. <b>2020</b> , 85, 1210-1219	2
1170	Synthesis of new $\pi$ -amino-1H indazolyl-phosphonate derivatives: Crystal structure, Hirshfeld surface analysis and DFT studies. <b>2020</b> , 1220, 128702	1
1169	Crystal structure and homopolar dihydrogen interactions in propano-bridged indigo. <b>2020</b> , 33, e4096	0
1168	Towards low-impact-sensitivity through crystal engineering: New energetic co-crystals formed between Picric acid, Trinitrotoluene and 9-Vinylanthracene. <b>2020</b> , 1219, 128614	5
1167	N-acetyl-5-isopropyl-2-tioximidazolidin-4-one: Synthesis, spectroscopic characterization, crystal structure, DFT calculations, Hirshfeld surface analysis and energy framework study. <b>2020</b> , 1219, 128630	2
1166	Synthesis, X-ray crystal structure elucidation and Hirshfeld surface analysis of -(4-(1-benzimidazole-2-yl)phenyl)carbamothioyl)benzamide: investigations for elastase inhibition, antioxidant and DNA binding potentials for biological applications.. <b>2020</b> , 10, 20837-20851	11
1165	Exploring intermolecular contacts in multi-substituted benzaldehyde derivatives: X-ray, Hirshfeld surface and lattice energy analyses.. <b>2020</b> , 10, 16861-16874	
1164	Intramolecular sp <sup>2</sup> -sp <sup>3</sup> 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. <b>2020</b> , 10, 369	2
1163	Synthesis, Single Crystal X-Ray Structure, Hirshfeld Surface Analysis, DFT Computations, Docking Studies on Aurora Kinases and an Anticancer Property of 3-(2,3-Dihydrobenzo[b][1,4]dioxin-6-yl)-6-methoxy-4H-chromen-4-one. <b>2020</b> , 10, 413	3
1162	Effects of Solvent and Reaction Time in Sonochemical Synthesis of Cadmium(II) Compounds and Use them as Template for Synthesis of Cadmium(II) Oxide Nano Structures. <b>2020</b> , 646, 1365-1372	1
1161	A Supramolecular Approach to Structure-Based Design with A Focus on Synthons Hierarchy in Ornithine-Derived Ligands: Review, Synthesis, Experimental and in Silico Studies. <b>2020</b> , 25,	14
1160	Towards white light emission from a hybrid thin film of a self-assembled ternary samarium(III) complex. <b>2020</b> , 44, 5673-5683	24
1159	Manganese tetraphenylporphyrin bromide and iodide. Studies of structures and magnetic properties. <b>2020</b> , 184, 114488	5
1158	Solid-State Landscape of 4,4'-Azobis(3,5-dimethyl-1H-pyrazole) with the Isolation of Conformer-Dependent Polymorphs. <b>2020</b> , 20, 2721-2733	1
1157	Exploring Ambipolar Semiconductor Nature of Binary and Ternary Charge-Transfer Cocrystals of Triphenylene, Pyrene, and TCNQ. <b>2020</b> , 124, 6544-6553	12
1156	Two-Dimensional Coordination Polymer {[Bi( $\mu$ -z)I <sub>3</sub> ]}: Structure and Analysis of the Packing Using the Hirshfeld Surface Method. <b>2020</b> , 46, 23-27	7



1155	Novel tris(5-aryl-1H-tetrazol-1-yl)methanes and 2-dichloromethyl-5-aryl-2H-tetrazoles and noncovalent interactions in their crystal structure. <b>2020</b> , 57, 2539-2547	2
1154	Structural characterization and Hirshfeld surface analysis of the pyrazoline 1-(3-(4-iodophenyl)-5-(3-methylthiophen-2-yl)-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one. <b>2020</b> , 1210, 128044	6
1153	Halogen Bonding Provides Heterooctameric Supramolecular Aggregation of Diaryliodonium Thiocyanate. <b>2020</b> , 10, 230	14
1152	Molecules Forced to Interact: Benzene and Pentafluoroiodobenzene. <b>2020</b> , 20, 3217-3223	2
1151	Crystal structures and Hirshfeld surface analysis of (cat) <sub>2</sub> [Fe <sup>III</sup> (B-dipic)(NCS) <sub>3</sub> ] and (cat)[Fe <sup>III</sup> (B-dipic)(H <sub>2</sub> O)(NCS) <sub>2</sub> ] (dipic = dipicolinate). <b>2020</b> , 183, 114529	2
1150	Structural studies of a manganese(III) complex with spin-crossover and thermochromic properties. <b>2020</b> , 22, 3221-3233	6
1149	Supramolecular Assembly of Metal Complexes by (Aryl)I <sup>+</sup> [Pt] Halogen Bonds. <b>2020</b> , 26, 7692-7701	35
1148	Melting point/solubility/structure correlations in chiral and racemic model cocrystals. <b>2020</b> , 22, 2766-2771	9
1147	Cocrystals/salt of 1-naphthaleneacetic acid and utilizing Hirshfeld surface calculations for acid/aminopyrimidine synthons. <b>2020</b> , 22, 2978-2989	15
1146	Structural study, spectroscopic characterization, thermal behavior, DFT calculations and antimicrobial properties of a new hybrid compound, (C <sub>7</sub> H <sub>9</sub> N <sub>2</sub> ) <sub>2</sub> [HgCl <sub>4</sub> ]·4H <sub>2</sub> O. <b>2020</b> , 73, 506-523	4
1145	Crystal, spectral characterization, molecular docking, Hirshfeld computational studies and 3D-energy framework analysis of a novel puckered compound (C <sub>14</sub> H <sub>15</sub> Cl O): 2-Chloro-3-phenyl-5,5-dimethylcyclohex-2-en-1-one. <b>2020</b> , 1210, 127979	6
1144	syn and anti polymorphs of 2,6-dimethoxy benzoic acid and its molecular and ionic cocrystals: Structural analysis and energetic perspective. <b>2020</b> , 1221, 128721	4
1143	A new hybrid compound based on mercury and 3,3'-diaminobiphenylsulfone studied by a combined experimental and theoretical approach. <b>2020</b> , 1220, 128760	4
1142	Synthesis, crystal structure, Hirshfeld surface analysis, DNA binding, DNA cleavage activity and molecular docking of a new Schiff base nickel(II) complex. <b>2021</b> , 39, 5224-5234	1
1141	Improving solubility and intrinsic dissolution rate of ofloxacin API through salt formation via mechanochemical synthesis with diphenic acid. <b>2020</b> , 1221, 128806	7
1140	3β-Acetoxy cholest-5-ene crystals: Catalytic synthesis, structural elucidation, contribution of intermolecular interactions and density functional theory calculations. <b>2020</b> , 1221, 128833	
1139	Synthesis, characterization, and crystal structure analysis of Zn(II) and Cd(II) coordination compounds containing 4-((pyridin-4-ylmethylene)amino)phenol Schiff-base ligand. <b>2020</b> , 1221, 128846	1
1138	Synthesis, DFT calculations, intermolecular interactions and third order nonlinear optical properties of new organoammonium tetrabromocadmiate (II): (C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> Cl) <sub>2</sub> [CdBr <sub>4</sub> ]·4H <sub>2</sub> O. <b>2020</b> , 1222, 128853	7

1137	Nature of fluorine interactions in wheel and axle topology based hexa-coordinated Sn(IV)-porphyrins: an experimental and theoretical analysis. <b>2020</b> , 22, 5049-5059	0
1136	Structural Elucidation of the Mechanism of Molecular Recognition in Chiral Crystalline Sponges. <b>2020</b> , 59, 17600-17606	14
1135	Molecular salt crystals with bis(head-to-tail) interionic complementary assembly for efficient organic THz generators. <b>2020</b> , 8, 10078-10085	5
1134	The relationship between Hirshfeld potential and cytotoxic activity: a study along a series of flavonoid and chromanone derivatives. <b>2020</b> , 76, 723-733	1
1133	Ligand Control of Room-Temperature Phosphorescence Violating Kasha's Rule in Hybrid Organic-Inorganic Metal Halides. <b>2020</b> , 32, 1454-1460	23
1132	Chlorine directed C <sub>11</sub> and C <sub>H</sub> ?Cl interactions in acridinium 3,5-dichlorosalicylate: Synthesis, X-ray diffraction and theoretical analysis. <b>2020</b> , 1220, 128759	1
1131	Supramolecular assemblies through hydrogen bonding and Br <sub>2</sub> nitro interactions in 4-bromoanilinium 2,4-dinitrobenzoate crystals. <b>2020</b> , 1221, 128788	
1130	Synthesis, crystal structure, hirshfeld surface analysis, DFT calculations, anti-diabetic activity and molecular docking studies of (E)-N <sub>1</sub> (5-bromo-2-hydroxybenzylidene) isonicotinohydrazide. <b>2020</b> , 1221, 128800	24
1129	Synthesis, intermolecular interactions and biological activities of two new organic-inorganic hybrids CHN <sub>2</sub> Br and CHN <sub>2</sub> Cl <sub>2</sub> HO. <b>2020</b> , 10, 5864-5873	3
1128	Synthesis and structural studies of 16-ferrocenemethyl-estra-1,3,5(10)-triene-3,17 $\beta$ -diol and its interaction with human serum albumin by fluorescence spectroscopy and in silico docking approaches. <b>2020</b> , 34, e5483	3
1127	Some new nanostructure zinc complex: Synthesis, spectral analyses, crystal structure, Hirshfeld surface analyses, antimicrobial/anticancer, thermal behavior and usage as precursor for ZnO nanostructure. <b>2020</b> , 110, 110642	10
1126	Zinc(II) Complexes with Amino Acids for Potential Use in Dermatology: Synthesis, Crystal Structures, and Antibacterial Activity. <b>2020</b> , 25,	20
1125	Green approach for fabrication of a novel Zn(II) supramolecular compound as new precursor to produce nano-sized Zinc(II) oxide: Crystallography, topology, Hirshfeld Surface Analysis and biological activities. <b>2020</b> , 1208, 127885	10
1124	The study of inter and intramolecular hydrogen bonds of NLO crystal melaminium hydrogen malonate using DFT simulation, AIM analysis and Hirshfeld surface analysis. <b>2020</b> , 25, 307-315	3
1123	Cobalt(II) coordination complex with 2,5-bis(pyridine-2-yl)-1,3,4-thiadiazole and thiocyanate as co-ligand: Synthesis, crystal structure, Hirshfeld surface analysis, spectroscopic, thermal and magnetic properties. <b>2020</b> , 1208, 127892	6
1122	Three Multi-Components Reaction: Synthesis and X-Ray Single-Crystal of Hydroacridinone-Based Hydrazino-S-Triazine Derivative as a New Class of Urease Inhibitor. <b>2020</b> , 10, 14	3
1121	Light- and temperature-assisted spin state annealing: accessing the hidden multistability. <b>2020</b> , 11, 3281-3289	13
1120	Intramolecular hydrogen bonding stabilizes trans-configuration in a mixed carbene/isocyanide PdII complexes. <b>2020</b> , 912, 121174	14

1119	Effect of the coordination of $\pi$ -acceptor 4-cyanopyridine ligand on the structural and electronic properties of -tetra-(methoxy) and -tetra-(chlorophenyl) porphyrin cobalt(ii) coordination compounds. Application in the catalytic degradation of methylene blue dye.. <b>2020</b> , 10, 6900-6918	16
1118	Molecular Self-Assembly in a Family of Oxo-Bridged Dinuclear Ruthenium(IV) Systems. <b>2020</b> , 20, 2044-2056	7
1117	Three supramolecular trinuclear nickel(II) complexes based on Salamo-type chelating ligand: syntheses, crystal structures, solvent effect, Hirshfeld surface analysis and DFT calculation. <b>2020</b> , 45, 279-293	66
1116	Phase transition in 2-nitroanilinium bisulphate. Graph-set analysis, spectroscopic and theoretical studies. <b>2020</b> , 1206, 127772	2
1115	Synthesis and characterization of Lanthanum(III) complexes containing 4,4,4-trifluoro-1-(naphthalen-2yl)butane-1,3-dionate. <b>2020</b> , 179, 114384	4
1114	Hirshfeld surface analysis, crystal structure and physicochemical studies of a new Zn(II) complex with the 2,6-dimethylpyrimidin-4-(1H)-one ligand. <b>2020</b> , 101, 106119	2
1113	Sustained-Release Dual-Drug Ternary Salt Cocrystal of Piperazine Ferulate with Pyrazinamide: Synthesis, Structure, and Hirshfeld Surface Analysis. <b>2020</b> , 20, 2064-2073	14
1112	Tuning Solid-State Luminescence in Conjugated Organic Materials: Control of Excitonic and Excimeric Contributions through $\pi$ -Stacking and Halogen Bond Driven Self-Assembly. <b>2020</b> , 21, 616-624	14
1111	Structural elucidation, theoretical insights and thermal properties of three novel multicomponent molecular forms of gallic acid with hydroxypyridines. <b>2020</b> , 1207, 127828	7
1110	The effect of hydrostatic pressure on melt-castable energetic materials bis-oxadiazole-bis-methylene dinitrate: A density functional theory study. <b>2020</b> , 308, 113840	2
1109	Chiral Stereoisomer Engineering of Electron Transporting Materials for Efficient and Stable Perovskite Solar Cells. <b>2020</b> , 30, 1905951	15
1108	Organic $\pi$ -Hole Containing Crystals with Enhanced Nonlinear Optical Response and Efficient Optical-to-THz Frequency Conversion. <b>2020</b> , 8, 1901840	10
1107	Understanding the Role of Water in Different Solid Forms of Avibactam Sodium and Its Affecting Mechanism. <b>2020</b> , 20, 1150-1161	8
1106	Supramolecular frameworks formed via hydrogen bonding and non-covalent interactions and interaction energy calculations of solvent coordinated cis-dioxomolybdenum(VI) complexes derived from ONO donor aroylhydrazone: Cytotoxicity studies. <b>2020</b> , 505, 119472	4
1105	Supramolecular solid-state architecture formed by co-crystallization of melamine and phenylacetic acid. <b>2020</b> , 1207, 127833	3
1104	A new 1D coordination polymer of triphenyl lead hydrosulfide: Synthesis and insights into crystal architecture and Hirshfeld surface analyses. <b>2020</b> , 1207, 127801	7
1103	Recurrent Supramolecular Motifs in a Series of Acid-Base Adducts Based on Pyridine-2,5-Dicarboxylic Acid N-Oxide and Organic Bases: Inter- and Intramolecular Hydrogen Bonding. <b>2020</b> , 20, 1738-1751	15
1102	Fluorinated Thiophene-Phenylene Co-Oligomers for Optoelectronic Devices. <b>2020</b> , 12, 9507-9519	14

1101	Hydrogen-Bonded Framework Isomers Based on Zr-Metal Organic Cage: Connectivity, Stability, and Porosity. <b>2020</b> , 20, 4127-4134	16
1100	Synthesis, crystal structure and molecular modeling of a novel Chalcone-Quinolone Hybrid. <b>2020</b> , 1217, 128355	2
1099	Synthesis, structure and biological activity of zinc(II) pincer complexes with 2,4-bis(3,5-dimethyl-1H-pyrazol-1-yl)-6-methoxy-1,3,5-triazine. <b>2020</b> , 508, 119627	13
1098	Structural studies of Trenbolone, Trenbolone Acetate, Hexahydrobenzylcarbonate and Enanthate esters. <b>2020</b> , 1212, 128127	7
1097	New Halogen Chalcone with Potential for Application in Biofuels. <b>2020</b> , 34, 5958-5968	6
1096	Exploring the Polymorphism of Drostanolone Propionate. <b>2020</b> , 25,	6
1095	Synthesis and Structure Insights of Two Novel Broad-Spectrum Antibacterial Candidates Based on (')-[(Heteroaryl)methylene]adamantane-1-carbohydrazides. <b>2020</b> , 25,	3
1094	2-Chloro-7-methyl-3-((4-((p-tolyloxy)methyl)-1H-1,2,3-triazol-1-yl)methyl) quinoline: Crystal structure, hydrogen bonding and anti-bacterial activity. <b>2020</b> , 1212, 128137	2
1093	Broad-band luminescence involving fluconazole antifungal drug in a lead-free bismuth iodide perovskite: Combined experimental and computational insights. <b>2020</b> , 237, 118354	4
1092	Fluoride Ion Interactions in Alkali-Metal Fluoride-Diol Complexes. <b>2020</b> , 59, 6631-6639	6
1091	Effect of Ligand Field Strength on the Spin Crossover Behaviour in 5-X-SalEen (X=Me, Br and OMe) Based Fe(III) Complexes. <b>2020</b> , 15, 1709-1721	8
1090	Effect of fluorination on the crystal and electronic structure of organometallic cyclopentadienyl-phenylenediamino-cobalt complexes. <b>2020</b> , 918, 121277	3
1089	Conformational and crystal structure of acyl thiourea compounds: The case of the simple (2,2-dimethyl-propionyl) thiourea derivative. <b>2020</b> , 1215, 128227	6
1088	Different Stoichiometric Ratios Realized in Energetic Energetic Cocrystals Based on CL-20 and 4,5-MDNI: A Smart Strategy to Tune Performance. <b>2020</b> , 20, 3826-3833	13
1087	Relevant Hole tetrel bonding interactions in ethyl 2-triazolyl-2-oxoacetate derivatives: Hirshfeld surface analysis and DFT calculations. <b>2020</b> , 22, 3567-3578	13
1086	Pillar[5]arene-based self-assembled linear supramolecular polymer driven by guest halogen-halogen interactions in solid and solution states. <b>2020</b> , 11, 3305-3312	12
1085	Crystal structures of two furazidin polymorphs revealed by a joint effort of crystal structure prediction and NMR crystallography. <b>2020</b> , 76, 322-335	6
1084	Influence of CBr/X (X = S, Cl, N, Pt/Pd) Interactions on the Molecular and Crystal Structures of Pt(II) and Pd(II) Complexes with Thiomorpholine-4-carbonitrile: Crystallographic, Thermal, and DFT Study. <b>2020</b> , 20, 3018-3033	2

1083	Synthesis, growth, Hirshfeld surface analysis and crystal structure of a pyridine based chalcone single crystal. <b>2021</b> , 35, 387-391	1
1082	Synthesis, Hirshfeld Surface Analysis and DFT Studies of Ethano-tetracyclic Tetracene Derivatives. <b>2021</b> , 51, 196-204	1
1081	Insights into the structure-property relationship of pharmaceutical co-crystals: Charge density and quantum chemical approaches. <b>2021</b> , 1224, 129270	0
1080	Structural characterization, computational, charge density studies of 2-chloro-3-(2-methoxy)-5,5-dimethyl-2-cyclohexenone. <b>2021</b> , 1225, 129116	3
1079	Cobalt(III) complex of substituted nalidixic acid: Synthesis, characterization (IR, UV, EPR), single crystal X-ray, antimicrobial activity, Hirshfeld surface analysis and molecular docking. <b>2021</b> , 1225, 129043	2
1078	Quantum chemical insight into molecular structure, NBO analysis of the hydrogen-bonded interactions, spectroscopic (FT-IR, FT-Raman), drug likeness and molecular docking of the novel anti COVID-19 molecule 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(4-fluorophenyl)acetamide - dimer. <b>2021</b> , 314, 118825	9
1077	Investigating structural aspects of Pyridopyrimidinone derivatives, an important precursor in medicinal chemistry. <b>2021</b> , 1224, 129040	2
1076	Synthesis, crystal structure, spectroscopic (FT-IR, UV-Vis, EPR) and Hirshfeld surface analysis studies of Zn(II)-benzoate coordination dimer. <b>2021</b> , 1223, 128943	2
1075	Theoretical and experimental assesment of structural, spectroscopic, electronic and nonlinear optical properties of two aroylhydrazone derivative. <b>2021</b> , 1223, 128982	
1074	Synthesis, structural elucidation, spectroscopic, Hirshfeld surface analysis and theoretical simulation of a new adeninium orthoperiodate (1)bis(hydrate) organic-organic hybrid crystals. <b>2021</b> , 1224, 129034	3
1073	Synthesis of Bis(2,2,3,3-tetrafluoro-1,4-butanedioxy)-2-trans-6-bis(4-fluorobenzyl)spirocyclotetraphosphazene: Structural Characterization, Biological Activity and DFT Studies. <b>2021</b> , 51, 235-250	9
1072	Diverse structural assemblies of a series of ninhydrin derivatives: Quantitative analyses from experimental and theoretical studies. <b>2021</b> , 1224, 128920	2
1071	Experimental and theoretical corroboration of antimicrobial and anticancer activities of two pseudohalides induced structurally diverse Cd (II)-Salen complexes. <b>2021</b> , 1225, 129189	6
1070	Development of new L- Serine Squarate single crystal: Growth, structure, Hirshfeld surface analysis with enrichment ratio of atomic contacts. <b>2021</b> , 1224, 129190	4
1069	Structural studies on two new phosphoramides with the same [OC4H8N]P(O) segment by means of single-crystal X-ray diffraction, Hirshfeld surface analysis and 3D energy framework approach. <b>2021</b> , 1223, 128942	1
1068	Thermal, optical, etching, structural studies and theoretical calculations of [1-(2,5-Dichloro-benzenesulfonyl)-piperidin-4-yl]-(2,4-difluoro-phenyl)-methanone oxime. <b>2021</b> , 1224, 129077	9
1067	Morphologically controlled eco-friendly synthesis of a novel 2D Hg(II) metal-organic coordination polymer: Biological activities and DFT analysis. <b>2021</b> , 1226, 129335	3
1066	Polymorphism in the metal-organic hybrid (PhCH2NEt3)2[CoBr4]: Synthesis, crystal structures and physico-chemical characterizations. <b>2021</b> , 514, 119997	5

- 1065 Synthesis and structural characterization of a novel Zn(II) metal organic complex (Zn-MOC) and elimination of highly consumed antibiotic; tetracycline from aqueous solution by their nanostructures photocatalyst under visible light. **2021**, 1228, 129448 4
- 1064 Synthesis, crystal structure, DFT studies and Hirshfeld surface analysis of novel isoxazole derivatives. **2021**, 1228, 129450 1
- 1063 Spectroscopic, Electrochemical, Magnetic and Structural Characterization of an Hexamethylenetetramine Co(II) Porphyrin Complex [Application in the Catalytic Degradation of Vat Yellow 1 dye. **2021**, 1231, 129676 3
- 1062 The role of sulfur interactions in crystal architecture: experimental and quantum theoretical studies on hydrogen, halogen, and chalcogen bonds in trithiocyanuric acid-pyridine N-oxide co-crystals. **2021**, 23, 324-334 6
- 1061 Synthesis, 2D NMR, crystal structure, Hirshfeld surface, stereochemical and DFT studies of 4,8,9,10-tetraaryl-1,3-diazaadamantan-6-one O-methoxy oximes. **2021**, 1229, 129653 2
- 1060 Crystal structure, theoretical and vibrational analysis of isostructural salts of l-arginine analogue, (S)-2-amino-3-guanidinopropanoic acid. **2021**, 1229, 129620 2
- 1059 Structural and energetics of weak non-covalent interactions in two chemically distinct classes of O/N-heterocycles: X-ray and theoretical exploration. **2021**, 1227, 129694 1
- 1058 DFT and IsoStar Analyses to Assess the Utility of  $\pi$ -and  $\pi$ -Hole Interactions for Crystal Engineering. **2021**, 22, 141-153 5
- 1057 Ring opening of 2,6-diaryl-3,5-diphenyl piperidine-4-one by acetic acid: Structural studies and Hirshfeld surface analysis of (E)-4-aryl-1,3-diphenylbut-3-en-2-ones. **2021**, 58, 502-514
- 1056 Spectral studies and crystal structures of molybdenum(VI) complexes containing pyridine or picoline as auxiliary ligands: interaction energy calculations and free radical scavenging studies. **2021**, 46, 241-253 0
- 1055 Supramolecular association and quantification of intermolecular interactions of 4'-functionalized 2,2':6,2'-terpyridines: Experimental observation and theoretical studies. **2021**, 1226, 129254 1
- 1054 The quest for a better understanding of ethanol coordination to magnesium and zinc porphyrin: A combined experimental and theoretical study. **2021**, 1230, 129646 0
- 1053 Structural and biological features of bismuth(III) halide complexes with heterocyclic thioamides. **2021**, 1227, 129730 5
- 1052 Synthesis, structural and spectroscopic properties of [NE[(2,4-dihydroxyphenyl)methylidene]-4-(4-fluorophenyl) piperazine-1-carbothiohydrazide] thiosemicarbazone and its terbium complex. **2021**, 123, 108351 1
- 1051 Solid-liquid equilibrium behavior and thermodynamic analysis of p-aminobenzoic acid using experimental measurement and molecular dynamic simulation. **2021**, 323, 114964 8
- 1050 Experimental and computational studies of di- $\pi$ -chlorido-bis[chlorido(1,10-phenanthroline- $\pi$ N,N $\pi$ )] nickel(II) NiCl<sub>2</sub>(H<sub>2</sub>O)(C<sub>12</sub>N<sub>2</sub>H<sub>8</sub>): Crystal structure, quantitative analysis of the intermolecular interactions and electronic properties. **2021**, 1227, 129576
- 1049 Bifurcated  $\pi$ -I $\cdots$ (N,O) Halogen Bonding: The Case of (Nitrosoguanidinate)Ni(II) Cocrystals with Iodine(I)-Based  $\pi$ -Hole Donors. **2021**, 21, 588-596 16
- 1048 Comparative Conformational Study of a New Terpenoid-like Chalcone. **2021**, 1228, 129743 3

1047	New copper(II) complexes with (Z)-N <sup>?</sup> -{(2-hydroxynaphthalen-1-yl)methylene}acetohydrazide]: X-ray structure, Hirshfeld analysis, X-band electron paramagnetic resonance spectra, TD-DFT calculations and superoxide dismutase mimetic activity. <b>2021</b> , 195, 114969	6
1046	Penta- and dinuclear carboxylate nickel(II) complexes with pyrazole-based ligands: Syntheses, magnetic properties and DFT calculations. <b>2021</b> , 195, 114971	2
1045	Investigation of Structure-Property Relationships of Three Nitroaromatic Compounds: 1-Fluoro-2,4,6-trinitrobenzene, 2,4,6-Trinitrophenyl Methanesulfonate, and 2,4,6-Trinitrobenzaldehyde. <b>2021</b> , 21, 243-248	8
1044	Evaluation of structural, spectroscopic, bonding and electronic properties of some organotin(IV)-phosphoric triamide complexes by using help of DFT, QTAIM and Hirshfeld surface investigations. <b>2021</b> , 1195, 113098	2
1043	Pivotal role of supramolecular interactions towards the stability of Na-1,2-bis(tetrazol-5-yl) ethene coordination polymer. <b>2021</b> , 1226, 129376	
1042	Synthesis, characterization and crystal structure of bis-(methylsulfonylmethyl) sulfone, a symmetric acyclic trisulfone. <b>2021</b> , 1230, 129655	1
1041	Structural, spectroscopic insights, and antimicrobial properties of mononuclear and dinuclear metal(II) carboxylate derivatives with metronidazole. <b>2021</b> , 194, 114931	0
1040	Examining the structure and intermolecular forces of thiazolium-based ionic liquids. <b>2021</b> , 327, 114800	5
1039	Fabrication of a new 2D Co(II)-organic framework tuned by semi-flexible dicarboxylate and 1,4-bis(4-pyridinylmethyl)piperazine ligands: Topology, DFT/UB3LYP calculations, Hirshfeld surface analysis and magnetic studies. <b>2021</b> , 1229, 129616	0
1038	Interplay of weak noncovalent interactions in alkoxybenzylidene derivatives of benzohydrazide and acetohydrazide: a combined experimental and theoretical investigation and lipoxygenase inhibition (LOX) studies. <b>2021</b> , 23, 955-971	5
1037	The syntheses of pyrazole amine substituted cyclotriphosphazenes: Spectroscopic and crystallographic characterizations. <b>2021</b> , 196, 168-175	1
1036	4-(3-Methoxyphenyl)-5-(2-thienylmethyl)-2,4-dihydro-3H-1,2,4-triazole-3-selone: Synthesis, structural characteristics and reactions. <b>2021</b> , 1227, 129537	1
1035	Spectroscopic, charge transfer interaction and docking studies of gardona insecticide. <b>2021</b> , 1227, 129557	1
1034	Dihydroquinoline derivative as a potential anticancer agent: synthesis, crystal structure, and molecular modeling studies. <b>2021</b> , 25, 55-66	5
1033	Cavitand and Flexible Amphiphilic Resorcin[4]arenes: Structural Characterization and Supramolecular Interactions in Crystal Networks. <b>2021</b> , 51, 98-107	2
1032	Dinuclear Complex of Cu(II) Containing Chloride and Methoxide as Bridging-Ligands: A New Crystal Structure and DFT Calculations. <b>2021</b> , 51, 1-8	
1031	Comparative study of the photophysical and crystallographic properties of 4-(9H-pyreno[4,5-d]imidazol-10-yl)phenol and its alkylated derivatives. <b>2021</b> , 45, 7647-7658	
1030	Fluorine as a robust balancer for tuning the reactivity of topo-photoreactions of chalcones and the photomechanical effects of molecular crystals. <b>2021</b> , 23, 5856-5868	5

1029	Crystal structure and Hirshfeld surface analysis of ethyl (4,4a)-2-methyl-5,8-dioxo-6-phenyl-4a,5,6,7,7a,8-hexa-hydro-4-furo[2,3-]iso-indole-4-carboxyl-ate. <b>2021</b> , 77, 86-90	
1028	Effect of molecular geometry and extended conjugation on the performance of hydrogen-bonded semiconductors in organic thin-film field-effect transistors. <b>2021</b> , 9, 10819-10829	0
1027	Predicting molecular isomerism of symmetrical and unsymmetrical N,N'-diphenyl formamidines in the solid-state: crystal structure, Hirshfeld surface analysis, pairwise interaction energy, and $\pi$ - $\pi$ and $\pi$ - $\pi$ correlations. <b>2021</b> , 23, 4459-4474	0
1026	Solid-State Conformational Flexibility at Work: Energetic Landscape of a Single Crystal-to-Single Crystal Transformation in a Cyclic Hexapeptoid. <b>2021</b> , 21, 897-907	3
1025	Molecular design principles of ionic liquids with a sulfonyl fluoride moiety. <b>2021</b> , 45, 2443-2452	6
1024	Crystal structure, Hirshfeld surface and reactivity of novel ligand-LAT1 derived from dehydroacetic acid: intermolecular interactions with SARS-Cov-2/main protease. <b>2021</b> , 715, 81-103	1
1023	Crystal structure, Hirshfeld surfaces computational study and physicochemical characterization of 2,5-di-tert-butylanilinium chloride: [C <sub>14</sub> H <sub>24</sub> N]Cl. <b>2021</b> , 75, 1893-1905	
1022	Crystal structure and halogen-hydrogen bonding of a Delphine reaction inter-mediate. <b>2021</b> , 77, 1-4	
1021	Crystal engineering with pyrazolyl-thiazole derivatives: structure-directing role of $\pi$ -stacking and $\pi$ -hole interactions. <b>2021</b> , 23, 3276-3287	12
1020	Two polymorphs of remdesivir: crystal structure, solubility, and pharmacokinetic study. <b>2021</b> , 23, 2923-2927	2
1019	Hirshfeld Surface Analysis and Interactions Energy Calculations of Metal (II) 4-Cyanobenzoate with Nicotinamide / N,N'-Diethylnicotinamide Complexes. 125-136	1
1018	A theoretical insight on the anion-anion interactions observed in the solid state structure of a hetero-trinuclear complex. <b>2021</b> , 23, 1429-1438	9
1017	In acid-aminopyrimidine continuum: experimental and computational studies of furan tetracarboxylate-2-aminopyrimidinium salt.. <b>2021</b> , 11, 21463-21474	4
1016	Crystal structure and Hirshfeld surface analysis of 3-amino-1-oxo-2,6,8-triphenyl-1,2,7,8-tetra-hydro-iso-quinoline-4-carbo-nitrile. <b>2021</b> , 77, 195-199	11
1015	Synthesis, crystal structure and antibacterial studies of dihydropyrimidines and their regioselectively oxidized products.. <b>2021</b> , 11, 6312-6329	3
1014	Conformational analysis of two new organotin(IV) structures completed with a CSD survey. <b>2021</b> , 77, 68-80	2
1013	The effect of tether groups on the spin states of iron(II)/bis[2,6-di(pyrazol-1-yl)pyridine] complexes. <b>2021</b> , 50, 7417-7426	1
1012	The comparative reactions of 2-cis-4-ansa and spiro cyclotetraphosphazenes with difunctional ligands: Structural and stereogenic properties, electrochemical, antimicrobial and cytotoxic activity studies. <b>2021</b> , 35, e6150	11



1011	2D and 3D silver-based coordination polymers with thiomorpholine-4-carbonitrile and piperazine-1,4-dicarbonitrile: structure, intermolecular interactions, photocatalysis, and thermal behavior. <b>2021</b> , 23, 4799-4815	1
1010	Synthesis, Spectroscopic Properties and Hirshfeld Surface Analysis of 3,14-Dimethyl-2,6,13,17-tetraazoniatricyclo(16.4.0.07,12)docosane Tetrachloride Tetrahydrate. <b>2021</b> , 33, 1861-1867	
1009	Synthesis, structure and the Hirshfeld surface analysis of three novel metal-tiron coordination complexes.. <b>2021</b> , 11, 10767-10776	3
1008	A systematic investigation on the impact of the level of oxidation at sulfur and the configuration of R/S-sulfoxide on the solid structure. <b>2021</b> , 23, 4181-4193	
1007	Crystal Polymorphism-dependent Fluorescence of Fluoroarene-substituted Anthracene Derivatives. <b>2021</b> , 50, 31-34	2
1006	Design, synthesis, and characterization of pyridine-containing organic crystals with different substitution positions using solvothermal method. <b>2021</b> , 23, 3152-3159	0
1005	Supramolecular self-assembly and perfected / property of 5-fluorouracil and ferulic acid on the strength of double optimized strategy: the first 5-fluorouracil-phenolic acid nutraceutical cocrystal with synergistic antitumor efficacy. <b>2021</b> , 146, 2506-2519	2
1004	Synthesis, X-Ray Crystallography, Theoretical Investigation and Optical Properties of 2-Chloro-N-(2,4-dinitrophenyl) Acetamide. <b>2021</b> , 51, 523	
1003	Crystal structure and Hirshfeld surface analysis of the hydro-chloride salt of 8-[4-[(6-phenyl-pyridin-3-yl)methyl]piperazin-1-yl]-3,4-di-hydro-quinolin-2(1)-one. <b>2021</b> , 77, 208-212	
1002	Crystal structure, Hirshfeld surface analysis and energy framework study of 6-formyl-7,8,9,11-tetra-hydro-5-pyrido[2,1-]quinazolin-11-one. <b>2021</b> , 77, 47-51	0
1001	Crystal structure, Hirshfeld surface analysis and DFT study of 1-ethyl-3-phenyl-1,2-di-hydro-quinoxalin-2-one. <b>2021</b> , 77, 18-22	3
1000	Crystallographic and spectroscopic characterization of 2-[(7-acetyl-4-cyano-6-hydroxy-1,6-dimethyl-8-phenyl-5,6,7,8-tetra-hydro-isoquinolin-3-yl)sulfanyl]-phenyl-acetamide <b>2021</b> , 77, 121-125	
999	Nickel(II) complexes based on dithiolate-polyamine binary ligand systems: crystal structures, hirshfeld surface analysis, theoretical study, and catalytic activity study on photocatalytic hydrogen generation. <b>2021</b> , 50, 5632-5643	3
998	Desolvation of dasatinib methanolate: an improved anhydrous polymorph. <b>2021</b> , 23, 4272-4283	3
997	A computational probe granting insight into intra and inter-stacking interactions in squaraine dye derivatives. <b>2021</b> , 23, 22404-22417	
996	2,2'-Bipyridyl-1,1'-dioxide based bismuth(III) bromide hybrids: studies on crystal structure and luminescence. <b>2021</b> , 23, 3744-3752	6
995	X-ray characterization, Hirshfeld surface analysis, DFT calculations, in vitro and in silico lipoyxygenase inhibition (LOX) studies of dichlorophenyl substituted 3-hydroxy-chromenones.	11
994	Crystal structure, DFT studies and thermal characterization of new luminescent stannate (IV) based inorganic-organic hybrid compound. <b>2021</b> , 1224, 129266	10

- 993 Role of hydrogen bonds and weak non-covalent interactions in the supramolecular assembly of 9-hydroxyeucalyptol: crystal structure, Hirshfeld surface analysis, and DFT calculations. **2021**, 27, 13 2
- 992 Design, crystal structure determination, molecular dynamic simulation and MMGBSA calculations of novel p38- $\alpha$  MAPK inhibitors for combating Alzheimer's disease. **2021**, 1-14
- 991 Potential Third-Order Nonlinear Optical Response Facilitated by Intramolecular Charge Transfer in a Simple Schiff Base Molecule: Experimental and Theoretical Exploration. **2021**, 6, 6185-6194 9
- 990 Crystal structure and Hirshfeld surface analysis of poly[[bis- $\mu$ -(1,3,5-oxadiazinane-3,5-di-yl)bis(carbamoyl-methano-ato)]nickel(II)tetra-potassium] 4.8-hydrate]. **2021**, 77, 298-304 1
- 989 Role of Perfluorophenyl Group in the Side Chain of Small-Molecule n-Type Organic Semiconductors in Stress Stability of Single-Crystal Transistors. **2021**, 12, 2095-2101 5
- 988 Structural and theoretical analysis of 2-chloro-4-nitroaniline and 2-methyl-6-nitroaniline salts. **2021**, 77, 125-136
- 987 Elaboration, Crystal Structure, Physicochemical Characterization and DFT Theoretical Calculation of a New Cd(II) Complex [C<sub>9</sub>H<sub>14</sub>N]<sub>2</sub>CdCl<sub>4</sub>. 1
- 986 Effect of ortho- and para-chlorine substitution on hydroxychlorochalcone. **2021**, 27, 65 2
- 985 Halogen-Bonding-Driven Self-Assembly of Solvates of Tetrabromoterephthalic Acid. **2021**, 11, 198 1
- 984 A redetermination of the structure and Hirshfeld surface analysis of poly[di-aquadi-hydroxido-tetra-kis-(nicotinato -oxide)tricopper(II)]. **2021**, 77, 309-313
- 983 Synthesis, crystal structure and Hirshfeld surface analysis of [bis-(di-phenyl-phosphan-yl)methane- $\mu$ -chloridobis-[2-(pyridin-2-yl)phenyl- $\mu$ ]]iridium(III). **2021**, 77, 217-221
- 982 Crystal Structures of New Ivermectin Pseudopolymorphs. **2021**, 11, 172 1
- 981 New Pharmaceutical Salts of Trazodone. **2021**, 26, 0
- 980 Structural insights into the biological activity of a thioxopyrimidine derivative. **2021**, 27, 73
- 979 Crystal exploring, Hirshfeld surface analysis, and properties of 4?-(furan-2-yl)-2,2':6',2'-terpyridine complexes of nickel (II): New precursors for the synthesis of nanoparticles. **2021**, 35, e6179 1
- 978 Crystal structure and Hirshfeld surface analysis of 4,5-di-bromo-6-methyl-2-phenyl-2,3,3a,4,5,6,7,7a-octa-hydro-3a,6-ep-oxy-1-isoindol-1-one. **2021**, 77, 237-241 1
- 977 First divalent copper complex of a terdentate thiosemicarbazido-pyrazoline derived from 2,4-pentanedione bis(thiosemicarbazone): Synthesis, structural characterisation and antimicrobial in vitro activity assessment. **2021**, 195, 114992 1
- 976 Facile synthesis of single-crystal of o-phenylene diamine dihydrochloride as a polychloride and fabrication of high-performance semiconductor thin film. **2021**, 112, 110758 6

975	Cyclometalated Platinum(II) Complexes with Nitrile and Isocyanide Ligands: Synthesis, Structure, and Photophysical Properties. <b>2021</b> , 91, 393-400	0
974	Revealing new non-covalent interactions in polymorphs and hydrates of Acyclovir: Hirshfeld surface analysis, NCI plots and energetic calculations. <b>2021</b> , 1197, 113133	4
973	Pentacoordinated Fe(III) complex containing the cis-N2O2 asymmetrical tetradentate Schiff base and p-Br-C6H4O- as ligands. Promising building block for the construction of dipolar DA architectures: Synthesis, characterization, spectroscopic, electrochemical and structural studies. <b>2021</b> , 1228, 129709	0
972	The crystal structures, Hirshfeld surface analyses and energy frameworks of 8-[1-[3-(cyclo-pent-1-en-1-yl)benz-yl]piperidin-4-yl]-2-meth-oxy-quinoline and 8-[4-[3-(cyclo-pent-1-en-1-yl)benz-yl]piperazin-1-yl]-2-meth-oxy-quinoline. <b>2021</b> , 77, 372-377	
971	Crystal structure of -butyl 4-[4-(4-fluoro-phen-yl)-2-methyl-but-3-yn-2-yl]piperazine-1-carboxyl-ate. <b>2021</b> , 77, 360-365	1
970	Weak Interactions in Cocrystals of Isoniazid with Glycolic and Mandelic Acids. <b>2021</b> , 11, 328	3
969	Synthesis, characterization, crystal structure, Hirshfeld surface analysis, and theoretical study on a N-heterocyclic carbene salt and two NHC-Palladium complexes. 1-12	
968	A Rapid Ultrasound Synthesis of Xanthenediones Catalyzed by Boric acid in Ethanol-Water Medium: Single Crystal, DFT and Hirshfeld Surface Analysis of Two Representative Compounds. <b>2021</b> , 1228, 129794	5
967	IDENTIFICATION OF SUPRAMOLECULAR DIMERS IN THE CRYSTAL STRUCTURE OF (Z)-1-(((5-FLUOROPYRIDIN-2-YL)AMINO)METHYLENE)NAPHTHALEN-2(1H)-ONE via C(sp <sup>2</sup> )-H...F HYDROGEN BONDING: A COMBINED EXPERIMENTAL AND THEORETICAL STUDY. <b>2021</b> , 62, 460-466	2
966	Crystal structure and Hirshfeld surface analysis of ()-3-methyl-4-(thio-phen-2-yl-methyl-idene)isoxazol-5(4)-one. <b>2021</b> , 77, 378-382	
965	Peripherally octamethyl zinc(II) phthalocyanines with various axial substituents. <b>2021</b> , 197, 115024	2
964	Crystal structure, Hirshfeld surface analysis and density functional theory study of 6-methyl-2-[(5-methyl-isoxazol-3-yl)meth-yl]-1-benzimidazole. <b>2021</b> , 77, 396-401	2
963	2,5-Dibromothiophenes: Halogen Bond Involving Packing Patterns and Their Relevance to Solid-State Polymerization. <b>2021</b> , 21, 2526-2540	4
962	Supramolecular Self-Assembly Built by Weak Hydrogen, Chalcogen, and Unorthodox Nonbonded Motifs in 4-(4-Chlorophenyl)-3-[(4-fluorobenzyl)sulfanyl]-5-(thiophen-2-yl)-4-1,2,4-triazole, a Selective COX-2 Inhibitor: Insights from X-ray and Theoretical Studies. <b>2021</b> , 6, 6996-7007	3
961	Coordination isomerism in spin crossover (SCO) materials. <b>2021</b> , 129, 145501	1
960	Enhancing Single-Crystal Dichroism of an Asymmetric Azo Chromophore by Perfluorophenyl Embraces and Boron Coordination. <b>2021</b> , 21, 3143-3147	1
959	Crystal Structure and Hirshfeld Surface Analysis of Trimethoxy(1-naphthyl)silane [Intermolecular Interactions in a One-Component Single-Crystalline Trimethoxysilane. <b>2021</b> , 647, 1053-1057	6
958	A comprehensive study of structural, non-covalent interactions and electronic insights into N-aryl substituted thiosemicarbazones via SC-XRD and first-principles DFT approach. <b>2021</b> , 1230, 129852	3

957	Polymorphs of 2-[2-[(2,6-dichlorophenyl)amino]phenyl]acetic acid (Diclofenac): Differences from crystallography, Hirshfeld surface, QTAIM and NCIPlots. <b>2021</b> , 544, 111119	2
956	Encapsulation Characteristics of Cavitant Type Tetrabromo-Functionalized Resorcin[4]arenes in the Crystal Structure. 1	
955	Structure and phase transition in 1-(diaminomethylene)thiourea-1-ium m-nitrobenzoate monohydrate and the structure of its anhydrous deuterated analogue. <b>2021</b> , 1230, 129626	4
954	A new tetra-kis-substituted pyrazine carb-oxy-lic acid, 3,3',3'',3'''-[[pyrazine-2,3,5,6-tetra-yltetra-kis(methyl-ene)]tetra-kis-(sulfanedi-yl)]tetra-propionic acid: crystal structures of two triclinic polymorphs and of two potassium-organic frameworks. <b>2021</b> , 77, 480-488	0
953	Coumarin-triazole hybrids: Design, microwave-assisted synthesis, crystal and molecular structure, theoretical and computational studies and screening for their anticancer potentials against PC-3 and DU-145. <b>2021</b> , 1230, 129899	4
952	Synthesis, crystal structure, computational studies and spectroscopic characterization of a hybrid material self-assembly from tetra(isothiocyanate)cobalt(II) anion and 1-(4-methoxyphenyl)piperazinium. <b>2021</b> , 1230, 129929	2
951	An insight into the anticancer potential of carbamates and thiocarbamates of 10-demethoxy-10-methylaminocolchicine. <b>2021</b> , 215, 113282	7
950	Crystal structure and Hirshfeld surface analysis of 2-[[7-acetyl-8-(4-chloro-phen-yl)-4-cyano-6-hy-droxy-1,6-dimethyl-5,6,7,8-tetra-hydro-isoquinolin-3-yl]sulfan-yl]-1(4-chloro-phen-yl)ethan-1-one. <b>2021</b> , 77, 527-531	
949	Sonication-assisted synthesis of a strawberry-like nano-structure triphenyltin(IV) adduct as precursor for preparation of nano-sized SnP2O7: Crystal structure and DFT calculations. <b>2021</b> , 1230, 129630	
948	Chiral Self-Sorting of Di-formylated N-Hetero-ortho-phenylene Hexamers by Macrocyclization with Aromatic Diamines. <b>2021</b> , 2021, 2736-2745	
947	Synthesis, X-ray, Hirshfeld surface analysis, exploration of DNA binding, urease enzyme inhibition and anticancer activities of novel adamantane-naphthyl thiourea conjugate. <b>2021</b> , 109, 104707	7
946	CrystalExplorer 3.1: a program for Hirshfeld surface analysis, visualization and quantitative analysis of molecular crystals. <b>2021</b> , 54, 1006-1011	344
945	Structural study and Hirshfeld surface analysis of (E)-4-(2-methoxy-benzyl-idene)-3-phenyl-isoxazol-5(4H)-one. <b>2021</b> , 77, 564-568	
944	Crystal structure, Hirshfeld surface analysis and inter-action energy calculation of 1-decyl-2,3-di-hydro-1-benzimidazol-2-one. <b>2021</b> , 77, 559-563	
943	(3a,4,5,6,7a)-4,5-Di-bromo-2-[4-(tri-fluoro-meth-yl)phen-yl]-2,3,3a,4,5,6,7,7a-octa-hydro-3a,6-ep-oxy-1-isoindol-1-one: crystal structure and Hirshfeld surface analysis. <b>2021</b> , 77, 466-472	1
942	Crystal structure and Hirshfeld surface analysis of [2-(1-benzimidazol-2-yl- $\pi$ -aniline- $\pi$ )-di-chlorido-zinc(II)]-di-methyl-formamide monosolvate. <b>2021</b> , 77, 491-494	0
941	Novel Dihydro-1,3,2H-benzoxazine Derived from Furfurylamine: Crystal Structure, Hirshfeld Surface Analysis, Photophysical Property, and Computational Study. <b>2021</b> , 11, 568	1
940	Invariant and Variable Supramolecular Self-Assembly in 6-Substituted Uracil Derivatives: Insights from X-ray Structures and Quantum Chemical Study. <b>2021</b> , 21, 3234-3250	0

939	Experimental and theoretical studies of the structural, vibrational and optical properties of a new hybrid material (C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> Cl) <sub>2</sub> SiF <sub>6</sub> . <b>2021</b> , 1232, 129990	1
938	Crystal structure of potassium hydrogen bis-(()-2-{4-[3-(thio-phen-3-yl)acrylo-yl]phen-oxy}acetate). <b>2021</b> , 77, 609-614	
937	Crystal structure and Hirshfeld surface analysis of 1-[(()-2-(5-chloro-2-hydroxy-phen-yl)hydrazin-1-yl-idene)naphthalen-2(1)-one. <b>2021</b> , 77, 672-676	
936	Crystal structure and Hirshfeld surface analysis of -[(()-2-hydroxy-phen-yl)methyl-idene]aniline -oxide. <b>2021</b> , 77, 596-599	
935	Phosphorus-nitrogen compounds: part 53-synthesis, characterization, cytotoxic and antimicrobial activity, DNA interaction and molecular docking studies of new mono- and dispirocyclotriphosphazenes with pendant arm(s). <b>2021</b> , 1	1
934	Crystal structure, Hirshfeld surface analysis and DFT study of -2-amino-5-methyl-phen-yl)-2-(5-methyl-1-pyrazol-3-yl)acetamide. <b>2021</b> , 77, 638-642	2
933	Crystal structure, endo/exodentate conformations, spectroscopic properties, and Hirshfeld surface analysis of two constrained cyclam compounds with bromides and hydrates. <b>2021</b> , 1232, 130011	3
932	Structural characterization, spectroscopic properties, and Hirshfeld surface analysis of two copper(II) complexes with 3,14-dimethyl and 3,14-diethyl-2,6,13,17-diazadiazoniatricyclo[16.4.0.07,12]docosa-2,13-diene. <b>2021</b> , 1231, 129897	1
931	Structural Insights of Three 2,4-Disubstituted Dihydropyrimidine-5-carbonitriles as Potential Dihydrofolate Reductase Inhibitors. <b>2021</b> , 26,	1
930	Synthesis, structure, Hirshfeld surface, DFT, and molecular docking studies of a new organic cocrystal: creatinine:2,3-pyridinedicarboxylic acid. <b>2021</b> , 34, e4247	
929	Polymorphic Cocrystals of the Antimalarial Drug Pyrimethamine: Two Case Studies. <b>2021</b> , 21, 3699-3713	4
928	Qualitative and Quantitative Study of Intermolecular Interactions in Imidazo[2,1-b] [1,3,4] Thiadiazoles. <b>2021</b> , 6, 4265-4272	0
927	Formation of a New Cocrystal Methyl-4-hydroxybenzoate:Urea and Its Structural and Thermal Properties. <b>2021</b> , 56, 2000223	
926	Crystal structure and Hirshfeld surface analysis of 2-[[7-acetyl-4-cyano-6-hydroxy-8-(4-methoxy-phen-yl)-1,6-dimethyl-5,6,7,8-tetrahydro-iso-quinolin-3-yl]sulfonyl]-phenol. <b>2021</b> , 77, 663-667	
925	Exploring weak intermolecular interactions in two bis-1,3,4-oxadiazoles derivatives: A combined X-ray diffraction, Hirshfeld surface analysis and theoretical studies. <b>2021</b> , 1232, 130030	4
924	Solvates of New Arylpiperazine Salicylamide Derivative-a Multi-Technique Approach to the Description of 5 HTR Ligand Structure and Interactions. <b>2021</b> , 22,	0
923	Functional substituted Cu(II) Schiff base complexes, syntheses, X-ray and theoretical characterizations, and investigations of their polyphenol oxidase- and peroxidase-like activities. <b>2021</b> , 1232, 129975	3
922	Structural insight from intermolecular interactions and energy framework analyses of 2-substituted 6,7,8,9-tetrahydro-11H-pyrido[2,1-b]quinazolin-11-ones. <b>2021</b> , 77, 416-426	0

921	Crystal structure and Hirshfeld surface analysis of 2-(2-oxo-3-phenyl-1,2,3,8a-tetra-hydro-quinoxalin-1-yl)ethyl acetate. <b>2021</b> , 77, 643-646	
920	Discussion on structural, optical, thermal, mechanical, dielectric and third-order NLO properties of 3-Nitroanilinium chloride single crystals for optoelectronic applications. <b>2021</b> , 32, 16421-16431	1
919	Antibacterial and cytotoxicity assay of two new Zn(ii)complexes: Synthesis, characterization, X-Ray structure, topology, Hirshfeld surface and thermal analysis. <b>2021</b> , 1231, 129947	2
918	Bis(2-methyl-pyridinium) tetra-chlorido-cuprate(II): synthesis, structure and Hirshfeld surface analysis. <b>2021</b> , 77, 726-729	2
917	Crystal structure, Hirshfeld surface analysis, inter-action energy, and DFT studies of cholesteryl hepta-noate. <b>2021</b> , 77, 686-691	
916	Crystal structure, Hirshfeld and electronic transition analysis of 2-[(1-benzimidazol-1-yl)meth-yl]benzoic acid. <b>2021</b> , 77, 755-758	1
915	Structural and vibrational characterization of 1-(diaminomethylene)-thiouren-1-ium 4-aminobenzoate. <b>2021</b> , 1234, 130181	1
914	Organic THz Generators: A Design Strategy for Organic Crystals with Ultralarge Macroscopic Hyperpolarizability. <b>2021</b> , 9, 2100324	3
913	Structural investigations into a new polymorph of FTCNQ: towards enhanced semiconductor properties. <b>2021</b> , 77, 426-434	0
912	Crystal structure and Hirshfeld surface analysis of dimethyl 5-[2-(2,4,6-trioxo-1,3-diazinan-5-yl-idene)hydrazin-1-yl]benzene-1,3-di-carboxyl-ate 0.224-hydrate. <b>2021</b> , 77, 759-764	
911	Crystal structure and magnetic study of the complex salt [RuCp(PTA)-CN-12][RuCp(PTA)][Re(NO)Br(EtOH)(MeOH)]. <b>2021</b> , 77, 749-754	1
910	Study of the synthesis, structural, vibrational and optical properties of the new compound: (C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> ) <sub>2</sub> TeCl <sub>6</sub> . Cl <sub>2</sub> . 1	
909	Solid state and solubility study of a potential anticancer drug-drug molecular salt of diclofenac and metformin. <b>2021</b> , 1234, 130166	3
908	Synthesis, crystal structure, Hirshfeld surface analysis and characterization of a new Cd(II) complex with the 4,4'-dimethyl-2,2'-dipyridine monodentate ligand. 1	
907	Investigation of intermolecular interactions between [Ho(H <sub>2</sub> O) <sub>8</sub> ] <sup>4+</sup> based 3D metal-organic supramolecular host and bipyridyl guest through crystal structure and Hirshfeld surface analysis. <b>2021</b> , 74, 1879-1890	1
906	In-silico methods of cocrystal screening: A review on tools for rational design of pharmaceutical cocrystals. <b>2021</b> , 63, 102527	4
905	Growth, structural, Hirshfeld surface analysis, DFT validation on the crystal structure of 1, 10-Phenanthrolin-1-ium-5,6-dione perchlorate monohydrate. <b>2021</b> , 33, 100706	0
904	Ultrasound-based synthesis, SC-XRD, NMR, DFT, HSA of new Schiff bases derived from 2-aminopyridine: Experimental and theoretical studies. <b>2021</b> , 1233, 130105	25

903	Structural, Hirshfeld surface studies and computation of interaction energies of 4-Amino-N-(3-chloropyrazin-2-yl)benzene-1-Sulfonamide organic compound. <b>2021,</b>	0
902	Spectroscopic (FT-IR, FT-Raman, UV-Vis) molecular structure, electronic, molecular docking, and thermodynamic investigations of indole-3-carboxylic acid by DFT method. <b>2021,</b> 1234, 130182	8
901	Ligand Steric Hindrances Switch Bridging (2-1)O <sub>2</sub> to Two-Center 1O Halogen-Bonding Mode in the Assembly of Diketonate Copper(II) Species. <b>2021,</b> 21, 4073-4082	3
900	Facile Synthesis, Crystal Structure, Spectral Characterization, Quantum Chemical Calculations, and Hirshfeld Surface Analysis of 5-Chloro-3-Methoxy-4-Hydroxybenzaldehyde. <b>2021,</b> 56, 2100017	
899	Advances in adsorptive separation of benzene and cyclohexane by metal-organic framework adsorbents. <b>2021,</b> 437, 213852	23
898	Syntheses and Structural Investigations of Penta-Coordinated Co(II) Complexes with -Pyrazolo-Triazine Pincer Ligands, and Evaluation of Their Antimicrobial and Antioxidant Activities. <b>2021,</b> 26,	2
897	Heteroleptic Cu(I) halide complexes with perchlorinated 1,10-phenanthroline. <b>2021,</b> 1234, 130199	4
896	Synthesis of 1-(2-Fluorophenyl)pyrazoles by 1,3-Dipolar Cycloaddition of the Corresponding Sydnone. <b>2021,</b> 26,	
895	Crystal structure, hirshfeld surface analysis and phase transformation behaviour of diisopropylammonium chloride hemihydrate crystals. <b>2021,</b> 153, 110008	1
894	Insights on a new sulfonamide chalcone with potential antineoplastic application. <b>2021,</b> 27, 211	1
893	Crystal structure and Hirshfeld surface analysis of ethyl 6'-amino-2'-(chloro-meth-yl)-5'-cyano-2-oxo-1,2-di-hydro-spiro-[indoline-3,4'-pyran]-3'-carboxyl-ate. <b>2021,</b> 77, 739-743	0
892	Synthesis, Characterization, and Properties of Rivaroxaban New Crystalline Forms. <b>2021,</b> 56, 2000243	0
891	Supramolecular architecture in sulfonylurea, sulfonyldiurea and sulfonyltriurea drugs: Synthesis, X-ray structure and Hirshfeld surface analysis. <b>2021,</b> 1233, 130158	
890	SolventAntisolvent Competitive Interactions Mediate Imidacloprid Polymorphs in Antisolvent Crystallization. <b>2021,</b> 21, 4318-4328	2
889	Syntheses, single crystal X-ray structure, Hirshfeld surface analyses, DFT computations and Monte Carlo simulations of New Eugenol derivatives bearing 1,2,3-triazole moiety. <b>2021,</b> 1234, 130189	6
888	High-Density Organic Electro-Optic Crystals for Ultra-Broadband THz Spectroscopy. <b>2021,</b> 9, 2100618	5
887	Crystal structure, Hirshfeld surface analysis and inter-action energy calculation of 4-(furan-2-yl)-2-(6-methyl-2,4-dioxo-pyran-3-yl-idene)-2,3,4,5-tetra-hydro-1-1,5-benzodiazepine. <b>2021,</b> 77, 834-838	
886	Tunable phase transition, band gap and SHG properties by halogen replacement of hybrid perovskites [(thiomorpholinium)PbX <sub>3</sub> , X = Cl, Br, I]. <b>2021,</b>	7

885	Crystal structure, spectral investigations, DFT and antimicrobial activity of brucinium benzilate (BBA). <b>2021</b> , 27, 223	3
884	Design and structural characterization of 2-methyl 8-hydroxyl quinolinium 5-chloro salicylate salt. 1-23	
883	Construction of Layered High-Energy Materials via Directional Hydrogen Bonding. <b>2021</b> , 21, 4725-4731	3
882	Combined DFT calculation, Hirshfeld surface analysis, and Energy framework study of non-covalent interactions in the crystal structure of (Z)-5-ethylidene-2-thiohydantoin determined by powder X-ray diffraction. <b>2021</b> , 1236, 130361	1
881	Development of Thiochroman Dioxide Analogues of Benzothiadiazine Dioxides as New Positive Allosteric Modulators of $\mu$ -Amino-3-hydroxy-5-methyl-4-isoxazolepropionic Acid (AMPA) Receptors. <b>2021</b> , 12, 2679-2692	3
880	Temperature-Triggered Supramolecular Assembly of Organic Semiconductors. <b>2021</b> , e2101487	2
879	Temperature and solvent dependent thermodynamic behavior of sulfathiazole. <b>2021</b> , 346, 117146	1
878	Molecular and Supramolecular Structures of Cd(II) Complexes with Hydralazine-Based Ligands; A New Example for Cyclization of Hydrazonophthalazine to Triazolophthalazine. <b>2021</b> , 11, 823	2
877	Structure analysis and evaluation of two probes for the colorimetric detection of Hg <sup>2+</sup> and turn-on fluorescence-based detection of Cd <sup>2+</sup> ions in an aqueous solution. <b>2021</b> , 1235, 130233	3
876	Azoimidazole gold(III) complexes: Synthesis, structural characterization and self-assembly in the solid state. <b>2021</b> , 522, 120373	8
875	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. <b>2021</b> , 1235, 130155	1
874	Crystal structure and physicochemical properties of a new optofunctional metal-organic cocrystal delivering intermolecular charge-transfer-enhanced nonlinear optical and optical limiting properties. <b>2021</b> , 32, 18669-18688	2
873	Crystal structure and Hirshfeld surface analysis of a pyrrolo-thia-zine complex. <b>2021</b> , 77, 770-774	
872	Corrosion inhibition performance of 4-(prop-2-ynyl)- [1,4]-benzothiazin-3-one against mild steel in 1 M HCl solution: Experimental and theoretical studies. <b>2021</b> , 46, 25800-25818	11
871	Synthesis, molecular docking, and in silico ADMET studies of 4-benzyl-1-(2,4,6-trimethyl-benzyl)-piperidine: Potential Inhibitor of SARS-CoV2. <b>2021</b> , 112, 104967	10
870	A Novel Centrosymmetric Fe(III) Complex with Anionic Bis-pyrazolyl-s-triazine Ligand; Synthesis, Structural Investigations and Antimicrobial Evaluations. <b>2021</b> , 13, 1247	1
869	Intramolecular Hydrogen Bond, Hirshfeld Analysis, AIM; DFT Studies of Pyran-2,4-dione Derivatives. <b>2021</b> , 11, 896	6
868	Design, synthesis, characterization, crystal structure, Hirshfeld surface analysis, DFT calculations, anticancer, angiogenic properties of new pyrazole carboxamide derivatives. <b>2021</b> , 1235, 130271	4



- 867 A New Insight into Non-covalent Interactions in 1,4-Disubstituted 1H-1,2,3-Triazole: Synthesis, X-ray structure, DFT calculations, in vitro Lipoxigenase Inhibition (LOX) and in silico Studies. **2021**, 1236, 130283 4
- 866 Crystal structure, Hirshfeld surface analysis and density functional theory study of benzyl 2-oxo-1-(prop-2-yn-1-yl)-1,2-di-hydro-quinoline-4-carboxyl-ate. **2021**, 77, 824-828
- 865 Design, synthesis, characterization, and antioxidant activity studies of novel thienyl-pyrazoles. **2021**, 7, e07592 5
- 864 Structural characterization and biological evaluation of antimony(III) and bismuth(III) complexes with imidazolidine-2-thione. **2021**, 1235, 130270 4
- 863 Synthesis, Crystal structure and Hirshfeld surface analysis of tetra[2,4-dichlorophenoxyacetate]cadmium(II) ethylenediamine 0.6H<sub>2</sub>O. **2021**, 34, 100712
- 862 Rationalizing the Formation of Belinostat Solvates with Experimental Screening and Computational Predictions. **2021**, 21, 4986-4996 0
- 861 One-Dimensional Hydrogen-Bonded NBD in the Hybrid Phosphate: Hirshfeld Surface Analysis and DFT Quantum Chemical Calculations. **2021**, 15, 359-368
- 860 Free radical scavenging activity and mechanisms of amidoalkyl-2-naphthol derivative: a joint experimental and theoretical study. **2021**, 75, 6651
- 859 Diaryliodonium Tetrachloroplatinates(II): Recognition of a Trifurcated Metal-Involving  $\pi\cdots\pi$ (Cl,Cl,Pt) Halogen Bond. **2021**, 21, 5360-5372 8
- 858 Interplay of Halogen and Hydrogen Bonding through Co-Crystallization in Pharmacologically Active Dihydropyrimidines: Insights from Crystal Structure and Energy Framework. **2021**, 86, 1167-1176 1
- 857 Easy preparation of novel 3,3-dimethyl-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide: Molecular structure, Hirshfeld surface, NCI analyses and molecular docking on AMPA receptors. **2021**, 1238, 130435 4
- 856 Crystal structure, Hirshfeld surface and photo-physical analysis of 2-nitro-3-phenyl-9-carbazole. **2021**, 77, 887-890 0
- 855 Crystal structure and Hirshfeld surface analysis of (0-1-[2,2-di-chloro-1-(4-methyl-phen-yl)ethen-yl]-2-(4-meth-oxy-phen-yl)diazene. **2021**, 77, 965-970 1
- 854 Influences of Chemical Functionalities on Crystal Structures and Electrochemical Properties of Dihydro-benzoxazine Dimer Derivatives. **2021**, 11, 979 0
- 853 Synthesis, structure analysis, DFT calculations, Hirshfeld surface studies, and energy frameworks of 6-Chloro-3-[(4-chloro-3-methylphenoxy)methyl][1,2,4]triazolo[4,3-b]pyridazine. **2021**, 1237, 130282 7
- 852 Architecting Layered Crystalline Organic Semiconductors Based on Unsymmetric  $\pi$ -Extended Thienoacenes. **2021**, 33, 7379-7385 6
- 851 A novel crystalline molecular salt of sulfamethoxazole and amantadine hybridizing antiviral-antibacterial dual drugs with optimal in vitro/vivo pharmaceutical properties. **2021**, 163, 105883 5
- 850 Synthesis, Single Crystal Structural Investigation, Hirshfeld Surface Analysis, Thermoanalysis and Spectroscopic Study of Two New Cu(II) and Co(II) Transition-Metal Complexes. **2021**, 11, 986 1

- 849 Crystal structure and Hirshfeld surface analysis study of ()-1-(4-chloro-phen-yl)--(4-ferrocenylphen-yl)methanimine. **2021**, 77, 875-879
- 848 Synthesis, crystal structure determination, Hirshfeld surface analysis, spectral characterization, theoretical and computational studies of titanium(IV) Schiff base complex. 1-19 3
- 847 Diastereomeric resolution of 3-chloromandelic acid with threo-(1S,2S)-2-amino-l-p-nitrophenyl-1,3-propanediol. **2021**, 33, 824-839
- 846 Hybrid of the 1,2,3-triazole nucleus and sesquiterpene skeleton as a potential antitumor agent: Hemisynthesis, molecular structure, Hirshfeld surface analysis, density functional theory, and in vitro cytotoxic and apoptotic effects. 8
- 845 Synthesis, structural analysis, Hirshfeld surface analysis, DFT calculations, in vitro and docking study on antioxidant activity of 6-chloro-3-[(4-methylphenoxy) methyl] [1,2,4] triazolo[4,3-b]pyridazine. 1-20 2
- 844  $\pi$ Noncovalent Interaction Involving 1,2,4- and 1,3,4-Oxadiazole Systems: The Combined Experimental, Theoretical, and Database Study. **2021**, 26, 12
- 843 Crystal structure of 9,9-di-ethyl-9-fluorene-2,4,7-tricarbaldehyde. **2021**, 77, 1029-1032
- 842 Metal-Involving Chalcogen Bond. The Case of Platinum(II) Interaction with Se/Te-Based  $\pi$ Hole Donors. **2021**, 143, 15701-15710 9
- 841 Structural variations of trinitrato(terpyridine)lanthanoid complexes. **2021**,
- 840 The competition between solvent $\pi$ solvent and solute $\pi$ solvent act on the nucleation process of 4-(methylsulfonyl)benzaldehyde. **2021**, 337, 116391 0
- 839 Crystallographic and Spectroscopic Investigations on Oxidative Coordination in the Heteroleptic Mononuclear Complex of Cerium and Benzoxazine Dimer. **2021**, 26, 1
- 838 The hydroxylic position mediated the luminescent properties based on 4-amino-4H-1,2,4-triazole: Syntheses, crystal structures and Hirshfeld analyses. **2021**, 301, 122300 1
- 837 Experimental and computational studies on the synthesis and structural characterization of 2-(4-chlorophenoxy)-N-[4-(4-methylphenyl)-1,3-thiazol-2-yl]acetamide. **2021**, 1249, 131588 1
- 836 Crystal structure, Hirshfeld surface analysis and density functional theory study of 1-nonyl-3-phenyl-quinoxalin-2-one. **2021**, 77, 1037-1042 0
- 835 Crystal structure and Hirshfeld surface analysis of ()-4-({2,2-di-chloro-1-[4-(di-methyl-amino)-phen-yl]ethenyl}diaz-en-yl)benzo-nitrile. **2021**, 77, 994-998
- 834 Side-group engineering of semiconducting naphthalene diimide derivatives with high solution-processability and high thermal stability. **2021**, 100, 106348 0
- 833 Investigation of stable solid diazonium salt by molecular structure, Hirshfeld surface analysis, optical and electrochemical studies, and applications. **2021**, 27, 296 2
- 832 Electronic property trends of single-component organic molecular crystals containing C, N, O, and H. **2021**, 197, 110510 0

831	Supramolecular Properties Directed by Weak Interactions in a Copper (II) Complex Based on 8-Hydroxy Quinoline-Pyridine Binary Ligand Systems: Crystal Structure and Hirshfeld Surface Analyses. 1	1
830	Parent B N -Perylenes with Different BN Orientations. <b>2021</b> , 60, 23313-23319	12
829	Parent B2N2-Perylenes with Different BN Orientations. <b>2021</b> , 133, 23501	0
828	Synthesis of novel benzohydrazide and benzoic acid derivatives: Crystal Structure, Hirshfeld surface analysis and DFT computational studies. <b>2021</b> , 1239, 130465	4
827	Exploring crystal structure of 5, 10, 15, 20-tetrakis (4-iodophenyl) porphyrin; H2TIPP: Experimental and theoretical investigations. <b>2021</b> , 1240, 130601	0
826	Crystal structure and Hirshfeld surface analysis of 2,2,2-tri-chloro-,bis-[[[(1,4)-1,4-di-hydro-1,4-ep-oxy-naphthalen-1-yl]meth-yl]acetamide. <b>2021</b> , 77, 1048-1053	
825	Copper(II) Complexes with NNN and NNO Schiff Base Ligands as Efficient Photodegradation Agents for Methylene Blue, Preferential BSA Binder and Biomaterial Transplants. <b>2021</b> , 113565	0
824	Defrasirox pyridine solvate and its Cu(II) complex: Synthesis, crystal structure, Hirshfeld surface analysis, antimicrobial assays and antioxidant activity. <b>2021</b> , 1249, 131525	1
823	Dimethyltin(IV) Coordination Polymers Featuring the Versatile Ligand of 2,2'-Bipyrimidine: A Multi-NMR, Hirshfeld Surface Analysis Study and Thermal Properties. 1	0
822	Synthesis, crystal structure elucidation, Hirshfeld surface analysis, 3D energy frameworks and DFT studies of 2-(4-fluorophenoxy) acetic acid. <b>2021</b> , 12, 304-313	1
821	New enaminone sesquiterpenic: TiCl <sub>4</sub> -catalyzed synthesis, spectral characterization, crystal structure, Hirshfeld surface analysis, DFT studies and cytotoxic activity. <b>2021</b> , 1241, 130622	13
820	Supramolecular architecture formed between amidinothiourea and 2-pyridinecarboxylic acid. <b>2021</b> , 1242, 130736	3
819	Design, Hemiynthesis, crystal structure and anticancer activity of 1, 2, 3-triazoles derivatives of totarol. <b>2021</b> , 115, 105165	15
818	Synthesis, structures, DFT calculations, and Hirshfeld surface analysis of sulfonium derivatives of the closo-decaborate anion [B <sub>10</sub> X <sub>9</sub> -cyclo-S(CH <sub>2</sub> ) <sub>4</sub> ] <sup>-</sup> and [B <sub>10</sub> X <sub>9</sub> -cyclo-S(CH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> O] <sup>-</sup> [X' = H, Cl, Br]. <b>2021</b> , 1241, 130591	8
817	Analyzing integrated C-H and hydrogen bonding interactions in N, N-Dimethyl-4-aminopyridinium benzilate. <b>2021</b> , 1242, 130717	1
816	New 1,2,3-triazole containing benzimidazolone derivatives: Syntheses, crystal structures, spectroscopic characterizations, Hirshfeld surface analyses, DFT calculations, anti-corrosion property anticipation, and antibacterial activities. <b>2021</b> , 1242, 130719	0
815	Decavanadate salts of piperidine and triethanolamine: A combined experimental and theoretical study. <b>2021</b> , 1241, 130677	2
814	Crystal structure, Hirshfeld surface analysis and DFT studies of Euphorbioside monohydrate a major bisnorsesquiterpene isolated from Euphorbia resinifera latex. <b>2021</b> , 1241, 130511	2

813	Examining the interactions of a thermally robust task-specific phosphonium-based ionic compound. <b>2021</b> , 35, 100760	1
812	Polymorphism in early development: The account of MBQ-167. <b>2021</b> , 608, 121064	
811	Synthesis, crystal structure characterization, Hirshfeld surface analysis, and Quantum chemical computations of Ethyl 5-(thiophene-2-carbonyl)thiazole-4-carboxylate. <b>2021</b> , 1242, 130747	4
810	Investigation on experimental and theoretical studies of NLO active organic single crystal: 3-methyl-1-[(2,3,5,6-tetramethylphenyl)methyl]piperidin-1-ium bromide. <b>2021</b> , 245, 167652	0
809	Synthesis, crystal structure, Hirshfeld surface analysis, DFT calculations, 3D energy frameworks studies of Schiff base derivative 2,2'-((1Z,1'Z)-(1,2-phenylene bis(azananylylidene)) bis(methanylylidene)) diphenol. <b>2021</b> , 1244, 130910	1
808	Unprecedented structural evidence for pyrrole-imine to azafulvene-amine tautomerization in iminopyrrolyl Schiff's base ligand: Coexistence of both tautomer's in a single crystal. <b>2021</b> , 1244, 131030	1
807	Spectroscopic characterization, X-ray molecular structures and cyclic voltammetry study of two (piperazine) cobalt(II) meso-arylporphyrin complexes. Application as a catalyst for the degradation of 4-nitrophenol. <b>2021</b> , 209, 115468	0
806	A new complex of Zinc (II) with sulfamethoxazole ligand: Synthesis, crystal structure, Hirshfeld surface analysis, thermal properties, DFT calculations and antibacterial/antifungal activities. <b>2021</b> , 1244, 130903	1
805	Synthesis, Characterization, Crystal Structure, Hirshfeld surface analysis and DFT studies of novel compounds based on the methoxynaphthalene ring. <b>2021</b> , 1244, 130947	0
804	Unusual mixed-valence CuI/CuI coordination polymer based on 2,5-bis(pyridine-2-yl)-1,3,4-thiadiazole and thiocyanate: Synthesis, structural characterization and antimicrobial in vitro activity assessment. <b>2021</b> , 209, 115494	0
803	Reactivity of the dodecahydro-closo-dodecaborate anion in zinc(II) and cadmium(II) complexation at the presence of azaheterocyclic ligands. <b>2021</b> , 527, 120587	3
802	Two exodentate conformations, spectroscopic properties, and Hirshfeld surface analysis of new macrocyclic compounds with tetrabromide and tetraperchlorate. <b>2021</b> , 1243, 130790	1
801	A combined experimental and theoretical analysis on the solid-state supramolecular assemblies of pent-2-ynol derivatives. <b>2021</b> , 1243, 130813	1
800	Bismuth(III) halide complexes of aromatic thiosemicarbazones: Synthesis, structural characterization and biological evaluation. <b>2021</b> , 208, 115388	5
799	Structural, spectroscopic studies, thermal proprieties and Hirshfeld surface analysis of a novel tetra-piperidinium disodium decavanadate nonahydrate. <b>2021</b> , 1244, 130969	1
798	Probing solvent effect and strong and weak interactions in 2-Nitrophenyl-hydrazine using independent gradient model and Hirshfeld from wave function calculation. <b>2021</b> , 341, 117345	1
797	Sonication-assisted synthesis of new Schiff bases derived from 3-ethoxysalicylaldehyde: Crystal structure determination, Hirshfeld surface analysis, theoretical calculations and spectroscopic studies. <b>2021</b> , 1243, 130782	14
796	Synthesis, X-ray crystallography, Hirshfeld surface analysis, thermal properties and DFT/TD-DFT calculations of a new material hybrid ionic (C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O <sub>8</sub> ·2ClO <sub>4</sub> ·4H <sub>2</sub> O). <b>2021</b> , 1244, 130955	1

795	Novel bisthiazole ligand and its copper(II) complex with unusual seven membered ring: Synthesis, characterization, experimental and theoretical study of the effect of ligand flexibility, and antimicrobial activity. <b>2021</b> , 209, 115490	2
794	Synthesis, characterization and DFT calculated properties of electron-rich hydrazinylthiazoles: Experimental and computational synergy. <b>2021</b> , 1245, 131043	6
793	Synthesis, characterization, $^{31}\text{P}\{^1\text{H}\}$ NMR, X-ray structure and voltammetric study of 2-mercaptothiazolines and phosphines ruthenium(II) complexes. <b>2021</b> , 1246, 131262	
792	Solid-liquid phase equilibrium of N, N'-diphenyl thiourea (DPTU) in twelve pure solvents: Solubility determination, correlation, molecular simulation and thermodynamic analysis. <b>2021</b> , 163, 106605	1
791	Intra- and intermolecular $\text{NH}\cdots\text{C}$ hydrogen bonds in 1-acyl urea compounds: Synthesis, X-ray structure, conformational and Hirshfeld surface analyses of 1-(2,3-dichlorophenyl)-3-pivaloylurea. <b>2021</b> , 1245, 131271	2
790	Comprehensive investigation of structural properties (X-ray diffraction, IR, Hirshfeld, MEP and FMOs) and in silico screening of potential biological activity of Euphorbia factor L1. <b>2021</b> , 1246, 131237	1
789	Crystal structure, Hirshfeld surface analysis and DFT studies of N-(4-acetylphenyl)quinoline-3-carboxamide. <b>2021</b> , 1246, 131162	1
788	Synthesis, crystal structure, DFT studies, Hirshfeld surface analysis and drug delivery performance of bis(2-chloro-4,6-diaminopyrimidine)copper(II)-dichloride. <b>2021</b> , 1246, 131142	2
787	Crystal structure, Hirshfeld surface analysis and physicochemical studies of a new copper coordination polymer with 3,3'-diaminodiphenylsulfone as ligand. <b>2021</b> , 1245, 131236	1
786	Supramolecular, spectroscopic and computational analysis of weak interactions in some thiosemicarbazones derived from 5-acetylbarbituric acid. <b>2021</b> , 1245, 131031	0
785	Synthesis, molecular structure, DFT studies, in silico docking and molecular dynamics simulations of 2,6 dimethoxychalcone derivatives as BRD4 inhibitors. <b>2021</b> , 1245, 131032	1
784	3-(1,3-Dioxoisindolin-2-yl)-N,N-dimethylpropan-1-ammonium perchlorate: Synthesis, crystal structure, docking study and in vitro anticancer activity against the human hepatomas cell line (Hep G2). <b>2021</b> , 1245, 131006	0
783	Preparation of a novel solid acid bearing sulfur-containing active groups and evaluation of its activity for cellulose hydrolysis. <b>2021</b> , 224, 107004	0
782	Synthesis, crystal structure characterization, DFT calculations, Hirshfeld surface analysis and 3D energy frameworks of triazole pyridazine derivatives: Theoretical and experimental studies. <b>2021</b> , 1246, 131242	4
781	Synthesis, structure, optical and thermal analysis of the new compound of the new compound organo-metallic $(\text{C}_5\text{H}_6\text{N})_2\text{TeCl}_6$ . <b>2022</b> , 1247, 131282	
780	Synthesis, spectroscopic characterization, crystal structure, Hirshfeld surface analysis, linear and NLO properties of new hybrid compound based on tin fluoride oxalate and organic amine molecule $(\text{C}_{12}\text{N}_2\text{H}_9)_2[\text{SnF}_2(\text{C}_2\text{O}_4)_2]\cdot 2\text{H}_2\text{O}$ . <b>2022</b> , 1248, 131392	1
779	Molecular structure and DFT calculations of aqua(5,10,15,20-tetrakis[4-(benzoyloxy)phenyl]porphyrinato)magnesium-dioxane. <b>2022</b> , 1248, 131469	0
778	Performance of copper(II)-azide with hydrogen bonding as initiating explosive. <b>2022</b> , 429, 132186	1

- 777 Synthesis, spectroscopic characterization, crystal structure, DFT, ESI-MS studies, molecular docking and in vitro antibacterial activity of 1,5-benzodiazepin-2-one derivatives. **2022**, 1247, 131188 1
- 776 Zinc(II) complexes constructed from an adamantane-functionalized pyridine Schiff base - Influence of the counterion on the supramolecular organization by means of C-H...O, C-H...N, C-H... $\pi$  and  $\pi$ - $\pi$  interactions. **2022**, 1247, 131241 1
- 775 Low pH-induced lone-pair activity in the hybrid (C<sub>6</sub>H<sub>10</sub>N<sub>2</sub>)[SnCl<sub>3</sub>]Cl: Chemical study and physical characterizations. **2022**, 1248, 131403 1
- 774 Synthesis, characterization, crystal and molecular structure and theoretical study of N-(naphthalen-1-yl)-2-(piperidin-1-yl) acetamide, a selective butyrylcholinesterase inhibitor. **2022**, 1248, 131544 1
- 773 Joint experimental and computational studies of a cyanomethylcarbonyl-bridged pyrene-dinitrobenzene molecular ensemble. **2022**, 1247, 131374 0
- 772 Crystal structure analysis of three (E)-N-(3-methyl, 5-fluorophenyl)-2-(4-substituted benzylidene)thiosemicarbazone derivatives: Experimental and theoretical studies. **2022**, 1247, 131383 1
- 771 Isomeric nitro substituted symmetrical benzamides: Crystal Structures, Hirshfeld surface analysis, 3D energy frameworks, DNA binding and cell line studies. **2022**, 1247, 131396 1
- 770 [Diaquo{bis(p-hydroxybenzoato- $\eta$ O1)}(1-methylimidazole- $\eta$ N1)}copper(II)]: Synthesis, crystal structure, catalytic activity and DFT study. **2022**, 1247, 131323 0
- 769 Exploring packing features of N-substituted acridone derivatives: Synthesis and X-ray crystallography studies. **2022**, 1248, 131448 1
- 768 SCXRD, DFT and molecular docking based structural analyses towards novel 3-piperazin-1-yl-benzo[d]isothiazole and 3-piperidin-4-yl-benzo[d]isoxazoles appended to quinoline as pharmacological agents. **2022**, 1248, 131442 0
- 767 Synthesis, physicochemical properties, crystal molecular structure and DFT investigation of an organobismuth(III) bis(dimethyldithiocarbamate) and its organolithium precursor. **2022**, 1247, 131335 0
- 766 Insight into structural description of novel 1,4-Diacetyl-3,6-bis(phenylmethyl)-2,5-piperazinedione: synthesis, NMR, IR, Raman, X-ray, Hirshfeld surface, DFT and docking on breast cancer resistance protein. **2022**, 1248, 131435 2
- 765 Synthesis and structure of (E)-((4-methoxyphenyl)-2-[4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy]acetamide. **2021**, 77, 184-189 0
- 764 Polynuclear 2D Copper(II) Complex of Pyrazine Containing Perchlorate As a Counter-Ion: Crystal Structure and DFT Calculations. **2021**, 4, 1-7 1
- 763 Photocatalytic activity of new nanostructures of an Ag(I) metal-organic framework (Ag-MOF) for the efficient degradation of MCPA and 2,4-D herbicides under sunlight irradiation. **2021**, 45, 3408-3417 20
- 762 Structure, intermolecular interactions, and dynamic properties of NTO crystals with impurity defects: a computational study. **2021**, 23, 2455-2468 4
- 761 Phosphorus-nitrogen compounds. Part 54. syntheses of chiral amino-4-fluorobenzyl-spiro(N/O)cyclotriphosphazenes: structural and stereogenic properties. **2021**, 45, 12178-12192 6
- 760 High temperature anionic Fe(III) spin crossover behavior in a mixed-valence Fe(II)/Fe(III) complex. **2021**, 50, 5960-5967 2

759	Hydrogen bond synthons affect the coordination geometry of d10-metal halide complexes: synthetic methods, theoretical studies, and supramolecular architectures. <b>2021</b> , 23, 6276-6290	0
758	Cocrystals of Propylthiouracil and Nutraceuticals toward Sustained-Release: Design, Structure Analysis, and Solid-State Characterization. <b>2021</b> , 21, 1202-1217	13
757	Investigation of Solubility Behavior of Canagliflozin Hydrate Crystals Combining Crystallographic and Hirshfeld Surface Calculations. <b>2021</b> , 26,	1
756	Experimental and theoretical studies of 1,3,5-tris (bromomethyl)-2,4,6-trimethylbenzene with 2-pyridone. <b>2021</b> , 34, e4188	1
755	Coordination hydrogen bonds in the structures of different tris(pyridin-2-yl)phosphoric triamide derivatives.. <b>2021</b> , 11, 8178-8197	2
754	Synthesis and structural characterization of hexa-chlorido-oxido-tetra-kis-[[4-(phenyl-ethyn-yl)pyridine- $\pi$ ]-copper(II)] di-chloro-methane monosolvate. <b>2021</b> , 77, 42-46	
753	Insight into amoxicillin sodium heterosolvates and non-solvated form: crystal structures, phase transformation behaviors, and desolvation mechanism.	0
752	Microcrystal Electron Diffraction for Molecular Design of Functional Non-Fullerene Acceptor Structures. <b>2021</b> , 33, 966-977	5
751	Validation of the supramolecular synthon preference through DFT and physicochemical property investigations of pyridyl salts of organo-sulfonates. <b>2021</b> , 45, 4780-4790	7
750	Unravelling the fluorescence and semiconductor properties of a new coronene:TCNB charge transfer cocrystal polymorph.	2
749	Bifurcated Halogen Bonding Involving Diaryliodonium Cations as Iodine(III)-Based Double- $\pi$ -Hole Donors. <b>2021</b> , 21, 1136-1147	13
748	Coupling 6-chloro-3-methyluracil with copper: structural features, theoretical analysis, and biofunctional properties. <b>2021</b> , 50, 13533-13542	1
747	Crystal structure and hirshfeld surface analysis of 1, 2, 3, triazole bridged pyrrolizidine grafted macrocycle. <b>2020</b> , 28, 100427	2
746	Experimental and computational investigations of new indole derivatives: A combined spectroscopic, SC-XRD, DFT/TD-DFT and QTAIM analysis. <b>2020</b> , 1207, 127803	27
745	Crystal structure, Hirshfeld surface, DFT calculations and photophysical properties of 2,4,5-tris(4-pyridyl)imidazole hydrogen chloride. <b>2020</b> , 1213, 128175	1
744	Quantitative insights into the crystal structure of a mixed-ligand Co(III) complex: Experimental and theoretical studies. <b>2020</b> , 1216, 128207	14
743	New perovskite Ba <sub>0.7</sub> La <sub>0.3</sub> Ti <sub>0.55</sub> Fe <sub>0.45</sub> O <sub>3</sub> - $\beta$ prepared by citric sol-gel method: From structure to physical properties. <b>2020</b> , 1217, 128347	2
742	Regioselectivity of reduction of nitro groups in 3, 5-dinitrosalicylic acid monohydrate explored by experimental and theoretical charge density analysis. <b>2020</b> , 1217, 128483	1

- 741<sup>1</sup> Supramolecular networks in molecular complexes of pyridine boronic acids and polycarboxylic acids: synthesis, structural characterization and fluorescence properties. **2017**, 19, 3760-3775 17
- 740<sup>0</sup> Microwave assisted slurry conversion crystallization for manufacturing of new co-crystals of sulfamethazine and sulfamerazine. **2020**, 22, 1381-1394 3
- 739 A series of guanidine salts of 3,6-bis-nitroguanyl-1,2,4,5-tetrazine: green nitrogen-rich gas-generating agent.. **2020**, 10, 36287-36294 2
- 738<sup>8</sup> Synthesis, Structure, and Biological Assays of Novel Trifluoromethyl diazepine-Metal Complexes. **2020**, 73, 49 2
- 737 Molecular structure, DFT studies, Hirshfeld surface analysis, energy frameworks, and molecular docking studies of novel (E)-1-(4-chlorophenyl)-5-methyl-N-((3-methyl-5-phenoxy-1-phenyl-1H-pyrazol-4-yl)methylene)-1H-1, 2, 3-triazole-4-carbohydrazide. **2019**, 692, 83-93 13
- 736<sup>6</sup> Green synthesis of tetraketones: crystal structure, DFT studies and Hirshfeld surface analysis of 2,2'-((3,4-dimethoxyphenyl)methylene) bis(3-hydroxy-5,5-dimethylcyclohex-2-enone). **2020**, 709, 81-97 2
- 735 Synthesis, X-ray analysis and computational studies of two novel thiophene derivatives. **2020**, 41, 517-529 4
- 734<sup>4</sup> 1-Methyl-1-propyl-pyrrolidinium chloride. **2008**, 64, 0637 5
- 733 Atom interaction propensities of oxygenated chemical functions in crystal packings. **2017**, 4, 158-174 18
- 732<sup>2</sup> Protonated nucleobases are not fully ionized in their chloride salt crystals and form metastable base pairs further stabilized by the surrounding anions. **2018**, 5, 449-469 7
- 731<sup>1</sup> Crystal engineering of exemestane to obtain a co-crystal with enhanced urease inhibition activity. **2020**, 7, 105-112 1
- 730<sup>0</sup> Synthesis, crystallization, X-ray structural characterization and solid-state assembly of a cyclic hexapeptoid with propargyl and methoxyethyl side chains. **2017**, 73, 399-412 8
- 729 On the crystal structures and phase transitions of hydrates in the binary dimethyl sulfoxide-water system. **2020**, 76, 733-748 4
- 728<sup>8</sup> Five solvates of a multicomponent pharmaceutical salt formed by berberine and diclofenac. **2019**, 75, 1644-1651 2
- 727 Conformational flexibility in amidophosphoesters: a CSD analysis completed with two new crystal structures of (CHO)P(O)X [X = NHCH and N(CHCH)]. **2020**, 76, 104-116 3
- 726<sup>6</sup> N'-[(1E)-(5-Nitro-furan-2-yl)methylidene]thio-phene-2-carbohydrazide: crystal structure and Hirshfeld surface analysis. **2016**, 72, 1025-31 3
- 725<sup>5</sup> [2-trans-1,2-Bis-(pyridin-4-yl)ethene-(2) N:N']bis-[[1,2-bis-(pyridin-4-yl)ethene-(2) N:N']bis-[N-(2-hydroxy-eth-yl)-N-iso-propyl-dithio-carbamato-(2) S,S']cadmium} aceto-nitrile tetra-solvate: crystal structure and Hirshfeld surface analysis. **2016**, 72, 1085-92 10
- 724<sup>4</sup> Distinct coordination geometries in bis-[N,N-bis-(2-methoxy-eth-yl)di-thio-carbamato-(2) S,S']di-phenyltin(IV) and bis-[N-(2-methoxy-eth-yl)-N-methyl-dithio-carbamato-(2) S,S']di-phenyl-tin(IV): crystal structures and Hirshfeld surface analysis. **2016**, 72, 1130-7 6



723	[-Benzyl--(2-phenyl-ethyl)di-thio-carbamato- $\mu$ ]tri-phenyl-tin(IV) and [bis-(2-methoxy-ethyl)di-thio-carbamato- $\mu$ ]tri-phenyl-tin(IV): crystal structures and Hirshfeld surface analysis. <b>2016</b> , 72, 1480-1487	4
722	Crystal structure and Hirshfeld surface analysis of 2-[[2,8-bis-(tri-fluoro-methyl)quinolin-4-yl](hydroxy)methyl]piperidin-1-ium 2-hydroxy-2-phenyl-acetate hemihydrate. <b>2016</b> , 72, 1618-1627	8
721	Bis(-,di-ethyl-dithio-carbamato- $\mu$ )(3-hydroxy-pyridine- $\mu$ )zinc and bis-[-(2-hydroxy-ethyl)--methylthio-carbamato- $\mu$ ](3-hydroxy-pyridine- $\mu$ )zinc: crystal structures and Hirshfeld surface analysis. <b>2016</b> , 72, 1700-1709	3
720	Di-butyl-bis-[-(2-methoxy-ethyl)--methyl-dithio-carbamato- $\mu$ ]tin(IV): crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 260-265	10
719	Bis{4-methylbenzyl 2-[4-(propan-2-yl)benzylidene]hydrazine-carbodi-thio-ato- $\mu$ }nickel(II): crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 397-402	3
718	Bis[ $\mu$ -methyl-phenyl-dithio-carbamato- $\mu$ ]; $\mu'$ -bis-[-(methyl-phenyl-dithio-carbamato- $\mu$ )cadmium]: crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 429-433	1
717	-Di-chlorido-bis-(dimethyl sulfoxide- $\mu$ )bis-(4-fluoro-benzyl- $\mu$ )tin(IV): crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 667-672	8
716	2-[(4-Chloro-phenyl)selanyl]-3,4-dihydro-2-benzochromene-5,6-dione: crystal structure and Hirshfeld analysis. <b>2017</b> , 73, 918-924	3
715	Ethyl 2-(4-methoxy-phenyl)-6-oxa-3-aza-bicyclo[3.1.0]hexane-3-carboxyl-ate: crystal structure and Hirshfeld analysis. <b>2017</b> , 73, 1218-1222	6
714	1-{(0)-[(2)-3-(4-Methoxy-phenyl)-1-phenyl-prop-2-en-1-ylidene]amino}-3-phenyl-urea: crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 1607-1611	2
713	Crystal structures and Hirshfeld surfaces of differently substituted (0)-'benzylidene--methyl-2-(thio-phen-2-yl)acetohydrazides. <b>2017</b> , 73, 1636-1641	2
712	[ $\mu$ Bis(di-phenyl-phosphanyl)hexane]bis-[undeca-carbonyl--triruthenium(3-)] hexane monosolvate: crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 1652-1657	2
711	Green synthesis and crystal structure of 3-(benzothiazol-2-yl)thiophene. <b>2017</b> , 73, 1647-1651	3
710	A new monoclinic polymorph of -(3-methyl-phenyl)ethoxy-carbo-thio-amide: crystal structure and Hirshfeld surface analysis. <b>2017</b> , 73, 1889-1897	10
709	Crystal packing analysis of cryocrystallized 2,2,2-trifluoro-aceto-phenone. <b>2018</b> , 74, 607-612	3
708	3-{(0)-[4-(4-Hydroxy-3-methoxy-phenyl)butan-2-ylidene]amino}-1-phenyl-urea: crystal structure and Hirshfeld surface analysis. <b>2018</b> , 74, 21-27	2
707	Crystal structure and Hirshfeld surface analysis of aqua-bis-(nicotinamide- $\mu$ )bis-(4-sulfamoylbenzoato- $\mu$ )copper(II). <b>2018</b> , 74, 45-50	3
706	Crystal structure and Hirshfeld surface analysis of (0)-2-(5-bromo-2-hydroxy-benzylidene)hydrazine-carbo-thio-amide di-methyl sulfoxide monosolvate. <b>2018</b> , 74, 119-123	2

705	Bis(4-meth-oxy-chalcone 4-ethyl-thio-semi-carbazon-ato- $\eta^2$ )zinc(II): crystal structure and Hirshfeld surface analysis. <b>2018</b> , 74, 151-157	3
704	Crystal structure and Hirshfeld analysis of 2-(5-bromo-thio-phen-2-yl)aceto-nitrile. <b>2018</b> , 74, 189-192	1
703	Crystal structures and Hirshfeld surface analyses of bis- $\eta^2$ -bis-(2-meth-oxy-eth-yl)di-thio-carbamato- $\eta^2$ di-butyl-tin(IV) and $\eta^2$ -(2-meth-oxy-eth-yl)-methyl-dithio-carbamato- $\eta^2$ tri-phenyl-tin(IV). <b>2018</b> , 74, 302-308	4
702	Crystal structure and Hirshfeld surface analysis of di-aqua-bis-( $\eta^2$ -di-ethyl-nicotinamide- $\eta^2$ )bis-(2,4,6-tri-methyl-benzoato- $\eta^2$ )manganese(II). <b>2018</b> , 74, 422-427	4
701	Crystal structure, Hirshfeld surface analysis and anti-oxidant capacity of 2,2'-((1,1')-[1,2-phenyl-enebis(aza-nylyl-idene)])bis-(methanylyl-idene))bis-(5-benz-yloxy)phenol. <b>2018</b> , 74, 682-686	1
700	2-[(4-Chloro-phen-yl)sulfan-yl]-2-meth-oxy-1-phenyl-ethan-1-one: crystal structure and Hirshfeld surface analysis. <b>2018</b> , 74, 703-708	1
699	Crystal structure and Hirshfeld surface analysis of 4-phenyl-3-(thio-phen-3-ylmeth-yl)-1-1,2,4-triazole-5(4)-thione. <b>2018</b> , 74, 812-815	5
698	Crystal structure determination, Hirshfeld surface analysis and energy frameworks of 6-phenyl-sulfonyl-6-thieno[3,2-]carbazole. <b>2018</b> , 74, 878-883	4
697	4-(4-Acetyl-5-methyl-1-1,2,3-triazol-1-yl)benzo-nitrile: crystal structure and Hirshfeld surface analysis. <b>2018</b> , 74, 1195-1200	5
696	Crystal structure, Hirshfeld surface analysis and HOMO-LUMO analysis of (4-bromo-4-meth-oxy-benzyl-idene)benzohydrazide. <b>2018</b> , 74, 1500-1503	4
695	Crystal structure and Hirshfeld surface analysis of ethyl 2-{4-[(3-methyl-2-oxo-1,2-di-hydro-quinoxalin-1-yl)meth-yl]-1-1,2,3-triazol-1-yl}acetate. <b>2018</b> , 74, 1648-1652	2
694	Crystal structure and Hirshfeld surface analysis of (4-1-butyl-4-(2-oxo-propyl-idene)-2,3,4,5-tetra-hydro-1-1,5-benzodiazepin-2-one. <b>2018</b> , 74, 1669-1673	7
693	Crystal structure and Hirshfeld surface analysis of 1-[[2-oxo-3-(prop-1-en-2-yl)-2,3-di-hydro-1,3-benzo-diazol-1-yl]meth-yl]-3-(prop-1-en-2-yl)-2,3-di-hydro-1,3-benzo-diazol-2-one. <b>2018</b> , 74, 1746-1750	5
692	Crystal structure and Hirshfeld surface analysis of 1-[(1-butyl-1,2,3-triazol-4-yl)meth-yl]-3-methyl-quinoxalin-2(1)-one. <b>2018</b> , 74, 1815-1820	1
691	Crystal structure and Hirshfeld surface analysis of 2,4,6,11-tetra-kis-(4-fluoro-phen-yl)-9-oxa-1,5-di-aza-tri-cyclo-[5.3.1.0]undeca-ne. <b>2018</b> , 74, 1867-1871	1
690	Crystal structure and Hirshfeld surface analysis of 5-methyl-1,2,4-triazolo[1,5-]pyrimidine. <b>2018</b> , 74, 1833-1837	4
689	Crystal structure and Hirshfeld surface analysis of 1-benzyl-3-(prop-2-yn-1-yl)-2,3-di-hydro-1,3-benzo-diazol-2-one. <b>2018</b> , 74, 1842-1846	3
688	A 1:2 co-crystal of 2,2'-di-thiodi-benzoic acid and benzoic acid: crystal structure, Hirshfeld surface analysis and computational study. <b>2019</b> , 75, 1-7	11

- 687 Crystal structure and Hirshfeld surface analysis of 3,4-dihydro-2-(2,4-dioxo-6-methylpyran-3-ylidene)-4-(4-pyridin-4-yl)-1,5-benzodiazepine. **2019**, 75, 94-98 2
- 686 Synthesis, X-ray crystal structure, Hirshfeld surface analysis and DFT studies of ()'-(2-bromo-benzyl-idene)-4-methylbenzohydrazide. **2019**, 75, 109-114 2
- 685 Crystal structure and Hirshfeld surface analysis of ()-1-[2,2-di-chloro-1-(4-nitro-phen-yl)ethen-yl]-2-(4-fluoro-phen-yl)diazene. **2019**, 75, 237-241 13
- 684 Utilizing Hirshfeld surface calculations, non-covalent inter-action (NCI) plots and the calculation of inter-action energies in the analysis of mol-ecular packing. **2019**, 75, 308-318 233
- 683 Crystal structure and Hirshfeld surface analysis of a Schiff base: ()-6-[(5-chloro-2-meth-oxy-anilino)methyl-idene]-2-hy-droxy-cyclo-hexa-2,4-dien-1-one. **2019**, 75, 362-366 1
- 682 Crystal structure and Hirshfeld surface analysis of ()-1-(4-chloro-phen-yl)-2-[2,2-di-chloro-1-(4-fluoro-phen-yl)ethen-yl]diazene. **2019**, 75, 465-469 10
- 681 Crystal structure and Hirshfeld surface analysis of -2-[2-(4-chloro-phen-yl)-3,4-di-hydro-2-1-benzo-pyran-4-yl-idene]hydrazine-1-carbo-thio-amide. **2019**, 75, 707-710 1
- 680 Crystal structure and Hirshfeld surface analysis of 4-(2,6-di-chloro-benz-yl)-6-phenyl-pyridazin-3(2)-one. **2019**, 75, 650-654 2
- 679 Crystal structure, Hirshfeld surface analysis and inter-action energy and DFT studies of 3-((2)-2-[(2,4-di-chloro-phen-yl)methyl-idene]-3-oxo-3,4-di-hydro-2-1,4-benzo-thia-zin-4-yl}propane-nitrile. **2019**, 75, 721-727 12
- 678 Crystal structure and Hirshfeld surface analysis of ()-2-(2,4,6-tri-methyl-benzyl-idene)-3,4-di-hydro-naphthalen-1(2)-one. **2019**, 75, 746-750 3
- 677 Crystal structure, Hirshfeld surface analysis and HOMO-LUMO analysis of ()'-(3-hy-droxy-4-meth-oxy-benzyl-idene)nicotino-hydrazide monohydrate. **2019**, 75, 804-807 2
- 676 Crystal structure and Hirshfeld surface analysis of ()-6-[(2-hy-droxy-4-methyl-anilino)-methyl-idene]-4-methyl-cyclo-hexa-2,4-dien-1-one. **2019**, 75, 785-788 1
- 675 Crystal structures and Hirshfeld surface analyses of 4,4'-[[1,3-phenyl-enebis(methyl-ene)]bis(-oxy)]bis-(3-meth-oxy-benzaldehyde) and 4,4'-[[1,4-phenyl-ene-bis(methyl-ene)]bis(-oxy)]bis-(3-meth-oxy-benzal-de-hyde). **2019**, 75, 875-879 1
- 674 Crystal structure and Hirshfeld surface analysis of ()-6-[(2-hy-droxy-5-nitro-anilino)methyl-idene]-4-methyl-cyclo-hexa-2,4-dien-1-one. **2019**, 75, 812-815 3
- 673 Crystal structure and Hirshfeld surface analysis of ethyl 2-[5-(3-chloro-benz-yl)-6-oxo-3-phenyl-1,6-di-hydro-pyridazin-1-yl]acetate. **2019**, 75, 892-895 5
- 672 Crystal structure, DFT study and Hirshfeld surface analysis of ethyl 6-chloro-2-eth-oxy-quinoline-4-carboxyl-ate. **2019**, 75, 912-916 6
- 671 Some chalcones derived from thio-phen-3-carbaldehyde: synthesis and crystal structures. **2019**, 75, 957-963 7
- 670 Synthesis, crystal structure and Hirshfeld surface analysis of 2-chloro-3-[(2-phenyl-hydrazinyl-idene)meth-yl]quinoline. **2019**, 75, 964-968 2

669	Crystal structure and Hirshfeld surface analysis of (2)-3-(4-chloro-3-fluoro-phen-yl)-1-(3,4-di-meth-oxy-phen-yl)prop-2-en-1-one. <b>2019</b> , 75, 942-945	1
668	Crystal structure, Hirshfeld surface analysis and inter-action energy and DFT studies of 5,5-diphenyl-1,3-bis-(prop-2-yn-1-yl)imidazolidine-2,4-dione. <b>2019</b> , 75, 951-956	2
667	Crystal structures and Hirshfeld surface analysis of $[\eta\text{-}[(\text{CH})(\text{CHN})\text{P}]\text{Re}(\text{CO})\text{Br}]_2\text{CHCl}$ and the product of its reaction with piperidine, $[-\{(\text{CH})(\text{CHN})\text{P}\}(\text{CHN})\text{Re}(\text{CO})\text{Br}]$ . <b>2019</b> , 75, 1005-1010	1
666	Crystal structure of two '-(1-phenyl-benzyl-idene)-2-(thio-phen-3-yl)acetohydrazides. <b>2019</b> , 75, 1090-1095	2
665	Crystal structure and Hirshfeld surface analysis of 2-[(2-oxo-2-chromen-4-yl)-oxy]acetic acid dimethyl sulfoxide monosolvate. <b>2019</b> , 75, 1123-1127	1
664	Crystal structure, Hirshfeld surface analysis and corrosion inhibition study of 3,6-bis-(pyridin-2-yl)-4-[[{(3a,5,5a,8a,8b)-2,2,7,7-tetra-methyl-tetra-hydro-5-bis-[1,3]dioxolo[4,5-:4',5'-]pyran-5-yl)]meth-oxy]monohydrate. <b>2019</b> , 75, 1169-1174	1
663	Crystal structure and Hirshfeld surface analysis of a new di-thio-glycoluril: 1,4-bis-(4-meth-oxy-phen-yl)-3-methyl-tetra-hydro-imidazo[4,5-]imidazole-2,5(1,3)-di-thione. <b>2019</b> , 75, 1297-1300	4
662	Crystal structure and Hirshfeld surface analysis of bis-(benzoato- $\eta^1$ , $\eta^1$ )[bis-(pyridin-2-yl)-amine]nickel(II). <b>2019</b> , 75, 1301-1305	1
661	Synthesis and crystal structure of 1,3-bis-(4-hy-droxy-phen-yl)-1-imidazol-3-ium chloride. <b>2019</b> , 75, 1311-1315	1
660	Crystal structure, Hirshfeld surface analysis and DFT studies of 5-bromo-1-{2-[2-(2-chloro-eth-oxy)eth-oxy]eth-yl}indoline-2,3-dione. <b>2019</b> , 75, 1372-1378	1
659	Synthesis and redetermination of the crystal structure of salicyl-aldehyde (4)-morpholino-thio-semi-carbazone. <b>2019</b> , 75, 1389-1393	5
658	Crystal structure and Hirshfeld surface analysis of 2-hy-droxy-7-meth-oxy-1,8-bis-(2,4,6-tri-chloro-benzo-yl)naphthalene. <b>2019</b> , 75, 1418-1422	0
657	Crystal structure, Hirshfeld surface analysis and inter-action energy and DFT studies of 2-chloro-ethyl 2-oxo-1-(prop-2-yn-1-yl)-1,2-di-hydro-quinoline-4-carboxyl-ate. <b>2019</b> , 75, 1411-1417	2
656	Crystal structure and Hirshfeld surface analysis of (-but-yl)-2-(phenyl-ethyn-yl)imidazo[1,2-]pyridin-3-amine. <b>2019</b> , 75, 1564-1567	2
655	Crystal structure and Hirshfeld surface analysis of 2-amino-pyridinium hydrogen phthalate. <b>2019</b> , 75, 1627-1631	3
654	Crystal structure, DFT calculation, Hirshfeld surface analysis and energy framework study of 6-bromo-2-(4-bromo-phen-yl)imidazo[1,2-]pyridine. <b>2019</b> , 75, 1620-1626	11
653	Crystal structure and Hirshfeld surface analysis of 2-(4-nitro-phen-yl)-2-oxoethyl benzoate. <b>2019</b> , 75, 1719-1723	2
652	Crystal structures of two dimeric nickel di-phenyl-acetate com-plexes. <b>2019</b> , 75, 1768-1773	1

- 651 Crystal structure and Hirshfeld surface analysis of 2-(4-nitro-phen-yl)-2-oxoethyl picolinate. **2019**, 75, 1763-1767 1
- 650 Crystal structure, Hirshfeld surface analysis and DFT studies of ethyl 2-[4-[(2-eth-oxy-2-oxoeth-yl)(phen-yl)carbamo-yl]-2-oxo-1,2-di-hydro-quinolin-1-yl]acetate. **2019**, 75, 1753-1758<sup>T</sup>
- 649 Crystal structure and Hirshfeld surface analysis of a zinc xanthate complex containing the 2,2'-bi-pyridine ligand. **2019**, 75, 1857-1860 2
- 648 Crystal structure, Hirshfeld surface analysis and contact enrichment ratios of 1-(2,7-di-methyl-imidazo[1,2-]pyridin-3-yl)-2-(1,3-di-thio-lan-2-yl-idene)ethanone monohydrate. **2019**, 75, 1934-1939 2
- 647 Crystal structure, Hirshfeld analysis and a mol-ecular docking study of a new inhibitor of the Hepatitis B virus (HBV): ethyl 5-methyl-1,1-dioxo-2-[[5-(pentan-3-yl)-1,2,4-oxa-diazol-3-yl]meth-yl]-2-1,2,6-thia-diazine-4-carboxyl-ate. **2020**, 76, 12-17 1
- 646 Crystal structure, Hirshfeld surface analysis and DFT studies of 1-benzyl-3-[(1-benzyl-1,1,2,3-triazol-5-yl)meth-yl]-2,3-di-hydro-1,1,3-benzo-diazol-2-one monohydrate. **2020**, 76, 95-101 1
- 645 Crystal structure, spectroscopic characterization and Hirshfeld surface analysis of aqua-dichlorido-{{[pyridin-2-yl)methyl-idene]aniline}copper(II) monohydrate. **2020**, 76, 148-154 4
- 644 Crystal structure, Hirshfeld surface analysis and DFT studies of 1,3-bis-[2-meth-oxy-4-(prop-2-en-1-yl)phen-oxy]propane. **2020**, 76, 344-348 2
- 643 Crystal structure, Hirshfeld surface analysis and inter-action energy and DFT studies of 1-(1,3-benzo-thia-zol-2-yl)-3-(2-hy-droxy-eth-yl)imidazolidin-2-one. **2020**, 76, 370-376 1
- 642 Whole-mol-ecule disorder of the Schiff base compound 4-chloro--(4-nitro-benzyl-idene)aniline: crystal structure and Hirshfeld surface analysis. **2020**, 76, 417-422 2
- 641 A redetermination of the crystal structure of the mannitol complex NH[MoO(CHO)] $\cdot$ HO: hydrogen-bonding scheme and Hirshfeld surface analysis. **2020**, 76, 518-522 1
- 640 Crystal structure, Hirshfeld surface analysis and computational study of 2-chloro--[4-(methyl-sulfan-yl)phen-yl]acetamide. **2020**, 76, 594-598 2
- 639 Crystal structure and Hirshfeld surface analysis of diethyl 5-(2-cyano-phen-oxy)isophthalate. **2020**, 76, 905-908 1
- 638 Synthesis, crystal structure, DFT calculations and Hirshfeld surface analysis of 3-butyl-2,6-bis-(4-fluoro-phen-yl)piperidin-4-one. **2020**, 76, 651-655 6
- 637 Hydrogen-bonding patterns in 2,2-bis-(4-methyl-phen-yl)hexa-fluoro-propane pyridinium and ethyl-enedi-ammonium salt crystals. **2020**, 76, 742-746 1
- 636 Crystal structure and Hirshfeld surface analysis of 4-[2,2-di-chloro-1-[(1)-(4-fluoro-phen-yl)diazen-yl]ethen-yl]-,di-methyl-aniline. **2020**, 76, 811-815 3
- 635 Co-crystal structure, Hirshfeld surface analysis and DFT studies of 3,4-ethyl-ene-dioxy-thio-phen-ol solvated bis-[1,3-bis-(penta-fluoro-phen-yl)propane-1,3-dionato]copper(II). **2020**, 76, 820-825 1
- 634 Crystal structure and Hirshfeld surface analysis of 4-(naphthalen-2-yl)-[(1)-(4-propoxybenzyl-idene)]-1,3-thia-zol-2-amine. **2020**, 76, 920-923 2

633	Crystal structure, Hirshfeld surface analysis, inter-action energy and DFT studies of 4-[(4-allyl-2-meth-oxy-phen-oxy)meth-yl]-1-(4-meth-oxy-phen-yl)-1,2,3-triazole. <b>2020</b> , 76, 962-966	4
632	Crystal structure, Hirshfeld surface analysis and computational study of a rhodamine B-salicyl-aldehyde Schiff base derivative. <b>2020</b> , 76, 1027-1032	4
631	Phenol hemihydrate: redetermination of the crystal structure by neutron powder diffraction, Hirshfeld surface analysis and characterization of the thermal expansion. <b>2020</b> , 76, 1062-1069	1
630	Crystal structure and Hirshfeld surface analysis of the product of the ring-opening reaction of a di-hydro-benzoxazine: 6,6'-[(cyclo-hexyl-aza-nedi-yl)bis-(methyl-ene)]bis-(2,4-di-methyl-phenol). <b>2020</b> , 76, 1239-1244	1
629	Crystal structure and Hirshfeld surface analysis of ()-4-{2,2-di-chloro-1-[(3,5-di-methyl-phen-yl)diazen-yl]ethen-yl}-,di-methyl-aniline. <b>2020</b> , 76, 1251-1254	4
628	()-1-(2,6-Di-chloro-phen-yl)-2-(3-nitro-benzyl-idene)hydrazine: crystal structure and Hirshfeld surface analysis. <b>2020</b> , 76, 1291-1295	1
627	Crystal structures, Hirshfeld atom refinements and Hirshfeld surface analyses of tris-(4,5-di-hydro-furan-2-yl)methyl-silane and tris-(4,5-di-hydro-furan-2-yl)phenyl-silane. <b>2020</b> , 76, 1514-1519	2
626	Syntheses and crystal structures of hydrated and anhydrous 1:2 cocrystals of oxyresveratrol and zwitterionic proline. <b>2020</b> , 76, 1528-1534	2
625	Crystal structure and Hirshfeld surface analysis of (aqua- $\lambda$ -(methanol- $\lambda$ )-(2-oxido-benzyl-idene)threoninato- $\lambda$ ,' $\lambda$ )]copper(II). <b>2020</b> , 76, 1539-1542	0
624	Crystal structure, optical property and Hirshfeld surface analysis of bis-[1-(prop-2-en-1-yl)-1-imidazol-3-ium] hexa-chlorido-stannate(IV). <b>2020</b> , 76, 1624-1628	1
623	Crystal structure and Hirshfeld surface analysis of di-chlorido-(methanol- $\lambda$ )bis-(2-methyl-pyridine- $\lambda$ )copper(II). <b>2020</b> , 76, 1771-1774	1
622	Synthesis, Crystal Structure and Hirshfeld Surface Analysis of 3,14-Dimethyl-2,6,13,17-tetraazatricyclo(16.4.0.07,12)docosane-2-(nitric acid). <b>2020</b> , 32, 397-702	3
621	Three new amidophosphoric acid esters with a P(O)[OCH <sub>2</sub> C(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> O] segment: X-ray diffraction, DFT, AIM and Hirshfeld surface investigations of bi- and tri-furcated (three and four-center) hydrogen bond interactions. <b>2020</b> , 235, 69-84	1
620	Double Palindrome Water Chain in Cu(II) Theophylline Complex. Synthesis, Characterization, Biological Activity of Cu(II), Zn(II) Complexes with Theophylline. <b>2020</b> , 10, 97	4
619	Crystal Structures, Hirshfeld Surfaces, and Thermal Study of Isostructural Polymeric Ladders of La(III) and Sm(III) Coordination Compounds with 4,4'-Bipyridine and Dibromoacetates. <b>2020</b> , 13,	4
618	Three New Compounds Derived from Nitrofurantoin: X-Ray Structures and Hirshfeld Surface Analyses. <b>2015</b> , 05, 63-73	9
617	N-(Dibenzylcarbamothioyl)-3-methylbutanamide: Crystal structure, Hirshfeld surfaces and antimicrobial activity. <b>2017</b> , 8, 410-416	4
616	Stimuli-responsive temporary adhesives: enabling debonding on demand through strategic molecular design.. <b>2021</b> , 12, 15183-15205	3

- 615 Ionic indium(III) chloride hybrids incorporating a 2,2'-bipyrimidine ligand: studies on photoluminescence and structural transformation. **2021**, 50, 16406-16413 1
- 614 Synthesis, structure and biological evaluation of highly functionalized 2-azetidinone integrated spirooxindolopyrrolidine heterocyclic hybrid. **2022**, 1250, 131745
- 613 Synthesis, structural, spectral, antidiabetic, DNA interactions and molecular docking investigations of a piperidine derivative. **2022**, 1250, 131692 3
- 612 Photochemical Control of the Mechanical and Adhesive Properties of Crystalline Molecular Solids. 1
- 611 Cyclometalated Platinum(II)  $\beta$ -Diketonate Complexes with Extremely High External Quantum Efficiency for White Organic Light-Emitting Diodes. **2021**, 9, 2101233 5
- 610 Role of p in establishing the crystal structures of six hydrogen-bonded compounds of 4-methyl-quinoline with different isomers of chloro- and nitro-substituted benzoic acids. **2021**, 77, 1144-1152 0
- 609 Isoquinolinium 5-(2,4-di-nitro-phen-yl)-1,3-dimethyl-2,6-dioxo-1,2,3,6-tetra-hydro-pyrimidin-4-olate: crystal structure, Hirshfeld surface analysis and pharmacological evaluation. **2016**, 72, 570-4
- 608 (Tris{2-[(5-chloro-2-oxido-benzyl-idene)- $\beta$ -amino- $\beta$ -ethyl-yl]amine- $\beta$ -ytterbium(III)}: crystal structure and Hirshfeld surface analysis. **2016**, 72, 1390-1395 1
- 607 [-(4-Dec-yloxy-2-oxido-benzyl-idene)-3-hy-droxy-2-naphtho-hydrazidato- $\beta$ ]di-methyl-tin(IV): crystal structure and Hirshfeld surface analysis. **2017**, 73, 390-396 2
- 606 A triclinic polymorph of tri-cyclo-hexyl-phosphane sulfide: crystal structure and Hirshfeld surface analysis. **2017**, 73, 493-499
- 605 3-Hy-droxy-2-phenyl-2,3,3a,7a-tetra-hydro-1,5-pyrano[3,2-]pyrrol-5-one: crystal structure and Hirshfeld surface analysis. **2017**, 73, 746-751
- 604 Crystal structure and Hirshfeld surface analysis of di-aqua-bis-(isonicotinamide- $\beta$ -bis-(2,4,6-tri-methyl-benzoato- $\beta$ -nickel(II) dihydrate. **2017**, 73, 1237-1241
- 603 Crystal structure and Hirshfeld surface analysis of 2-amino-4-meth-oxy-6-methyl-pyrimidinium 2-hy-droxy-benzoate. **2017**, 73, 1305-1307 1
- 602 Supra-molecular patterns and Hirshfeld surface analysis in the crystal structure of bis-(2-amino-4-meth-oxy-6-methyl-pyrimidinium) isophthalate. **2017**, 73, 1595-1598
- 601 New monoclinic form of {-Ethyl -(4-nitro-phen-yl)thio-carbamato- $\beta$ -tri-4-tolyl-phosphane- $\beta$ -gold(I)}: crystal structure and Hirshfeld surface analysis. **2017**, 73, 1465-1471 4
- 600 Zwitterionic 1-((1)-[(4-hy-droxy-phen-yl)iminio]meth-yl)naphthalen-2-olate: crystal structure and Hirshfeld surface analysis. **2017**, 73, 1674-1678
- 599 -Benzyl 3-[1-(6-methyl-pyridin-2-yl)ethyl-idene]di-thio-carbazate: crystal structure and Hirshfeld surface analysis. **2018**, 74, 261-266 3
- 598 Crystal structures and Hirshfeld surfaces of two 1,3-benzoxa-thiol-2-one derivatives. **2018**, 74, 78-82 3

- 597 (1,2,5)-5-Methyl-2-[2-(4-nitro-phen-yl)propan-2-yl]cyclo-hexyl 2-(4-meth-oxy-phen-yl)-2,5-di-hydro-1-pyrrole-1-carboxyl-ate: crystal structure and Hirshfeld analysis. **2018**, 74, 414-418
- 596 Different mol-ecular conformations in the crystal structures of three 5-nitro-imidazolyl derivatives. **2018**, 74, 380-384
- 595 Synthesis, spectroscopic and Hirshfeld surface analysis and fluorescence studies of (2,2')-3,3'-(1,4-phenyl-ene)bis-[1-(4-hy-droxy-phen-yl)prop-2-en-1-one] , -di-methyl-formamide disolvate. **2018**, 74, 835-839
- 594 Crystal structure of ()'-[1-(4-amino-phen-yl)ethyl-idene]-2-hy-droxy-5-iodo-benzohydrazide methanol monosolvate. **2018**, 74, 910-914
- 593 Crystal structure and Hirshfeld surface analysis of (2)-3-(3-chloro-phen-yl)-1-(3,4-di-meth-oxy-phen-yl)prop-2-en-1-one. **2018**, 74, 935-938 3
- 592 Crystal structure and Hirshfeld surface analysis of 3,3',3''-[(1,3,5-triazine-2,4,6-tri-yl)tris(-oxy)]tris-(5,5-di-methyl-cyclo-hex-2-en-1-one). **2018**, 74, 1035-1038 2
- 591 Crystal structure and Hirshfeld surface analysis of (2)-3-(3-bromo-4-fluoro-phen-yl)-1-(3,4-di-meth-oxy-phen-yl)prop-2-en-1-one. **2018**, 74, 1063-1066 2
- 590 Crystal structure and Hirshfeld surface analysis of (2)-3-(2,4-di-chloro-phen-yl)-1-(2,5-di-chloro-thio-phen-3-yl)prop-2-en-1-one. **2018**, 74, 1201-1205 2
- 589 Multifunctional arylsulfonamide derivatives with 5-HT/5-HT receptor antagonistic activity: a structural study. **2018**, 74, 1477-1486 0
- 588 Crystal structure and Hirshfeld analysis of 2-[bis-(1-methyl-1-indol-3-yl)meth-yl]benzoic acid. **2018**, 74, 1580-1583
- 587 Crystal structure and Hirshfeld surface analysis of ()-4-chloro-'-(4-oxo-thia-zol-idin-2-yl-idene)benzene-sulfono-hydrazide monohydrate. **2018**, 74, 1569-1573
- 586 Crystal structure and Hirshfeld surface analysis of dimethyl (3a,6,6a,7)-2-(2,2,2-tri-fluoro-acet-yl)-2,3-di-hydro-1,6,7-3a,6:7,9a-di-epoxy-benzo[iso-quinoline-3a,6a-di-carboxyl-ate. **2018**, 74, 1599-1604
- 585 Crystal structure and Hirshfeld surface analysis of ()'-[4-(piperidin-1-yl)benzyl-idene]aryl-sulfono-hydrazides. **2018**, 74, 1826-1832
- 584 2-[[2,8-Bis(tri-fluoro-meth-yl)quinolin-4-yl](hy-droxy)meth-yl]piperidin-1-ium tri-chloro-acetate: crystal structure and Hirshfeld surface analysis. **2018**, 74, 1851-1856 3
- 583 A 1:2 co-crystal of 2,2'-thiodi-benzoic acid and tri-phenyl-phosphane oxide: crystal structure, Hirshfeld surface analysis and computational study. **2018**, 74, 1764-1771 8
- 582 2-((E)-{[3-(1H-Imidazol-1-yl)propyl]imino}methyl)-4-[(E)-(4-methylphenyl)diazenyl]phenol. **2019**, 4,
- 581 Crystal structure and Hirshfeld surface analysis of ()-3-(2-chloro-phen-yl)-1-(2,5-di-chloro-thio-phen-3-yl)prop-2-en-1-one. **2019**, 75, 124-128 1
- 580 Crystal structure and Hirshfeld surface analysis of a bromo-chalcone: ()-1-(3-bromo-phen-yl)-3-(2,6-di-chloro-phen-yl)prop-2-en-1-one. **2019**, 75, 264-267



- 579 Hydrogen-bonded mol-ecular salts of reduced benzo-thia-zole derivatives with carboxyl-ates: a robust (8) supra-molecular motif (even when disordered). **2019**, 75, 167-174 ○
- 578 Computational asymmetric catalysis: On the origin of stereoselectivity in catalytic reactions. **2019**, 53, 1-27 1
- 577 The crystal structures of benzyl-ammonium phenyl-acetate and its hydrate. **2019**, 75, 194-201
- 576 Crystal structure and Hirshfeld surface analysis of (2)-1-(3-bromo-phen-yl)-3-(4-fluoro-phen-yl)prop-2-en-1-one. **2019**, 75, 146-149
- 575 Synthesis, crystal structure and Hirshfeld surface analysis of 3-(4,4-dimethyl-2,3,4,5-tetra-hydro-1-1,5-benzodiazepin-2-yl-idene)-6-methyl-3,4-di-hydro-2-pyran-2,4-dione. **2019**, 75, 228-232 1
- 574 Crystal structure and Hirshfeld surfaces analysis of the nickel(II) complex of the Schiff base ligand 6,6'-((1,1')-[ethane-1,2-diylbis(aza-nylyl-idene)]bis-(methanylyl-idene))bis-[2-(tri-fluoro-meth-oxy)phenol]. **2019**, 75, 328-331 1
- 573 Crystal structure, Hirshfeld surface analysis and frontier mol-ecular orbital analysis of ()-4-bromo-'-(2,3-di-chloro-benzyl-idene)benzohydrazide. **2019**, 75, 324-327 1
- 572 Crystal structure, Hirshfeld surface analysis and DFT study of (2)-2-(4-fluoro-benzyl-idene)-4-(prop-2-yn-1-yl)-3,4-di-hydro-2-1,4-benzo-thia-zin-3-one. **2019**, 75, 372-377 5
- 571 Ethyl 2-(4-benzyl-3-methyl-6-oxo-1,6-dihydropyridazin-1-yl)acetate: crystal structure and Hirshfeld surface analysis. **2019**, 75, 392-396
- 570 Crystal structure of 3-meth-oxy-4-[2-(thia-zol-2-yl)diazen-1-yl]aniline monohydrate. **2019**, 75, 354-357 ○
- 569 Crystal structure and Hirshfeld surface analysis of two 5,11-methano-benzo[[1,2,4]triazolo[1,5-][1,3,5]oxa-diazo-cine derivatives. **2019**, 75, 492-498 ○
- 568 Crystal structure and Hirshfeld surface analysis of 2-(1-indol-3-yl)ethanaminium acetate hemihydrate. **2019**, 75, 451-455 ○
- 567 Crystal structure and Hirshfeld surface analysis of dimethyl (1\*,3a\*,3a\*,6a\*,9\*,9a\*)-3a,5,6,9a-tetra-hydro-1,4,9-1,3a:6a,9-di-epoxy-phenalene-2,3-di-carboxyl-ate. **2019**, 75, 460-464
- 566 Qu-anti-tative analysis of weak non-covalent inter-actions in ()-3-(4-chloro-phen-yl)-2-phenyl-acrylo-nitrile: insights from and Hirshfeld surface analysis. **2019**, 75, 499-505
- 565 The crystal structures of two new coumarin derivatives: 2-(4-{2-[(2-oxo-2-chromen-4-yl)-oxy]acet-yl}piperazin-1-yl)acetamide and -(2,4-di-meth-oxy-benz-yl)-2-[(2-oxo-2-chromen-4-yl)-oxy]acetamide. **2019**, 75, 482-488 1
- 564 Crystal structure, Hirshfeld surface analysis and DFT study of (2)-2-(2,4-di-chloro-benzyl-idene)-4-[2-(2-oxo-1,3-oxazolidin-3-yl)eth-yl]-3,4-di-hydro-2-1,4-benzo-thia-zin-3-one. **2019**, 75, 593-599 5
- 563 Crystal structure and Hirshfeld surface analysis of ()-2-[1-hy-droxy-2-(pyridin-2-yl)eth-yl]-4-[2-(4-meth-oxy-phen-yl)diazen-1-yl]phenol. **2019**, 75, 600-603
- 562 Crystal structure and Hirshfeld surface analysis of 3-(4-meth-oxy-phen-yl)-1-methyl-4-phenyl-1-pyrazolo-[3,4]pyrimidine. **2019**, 75, 638-641 ○



- 543 Synthesis, crystal structure and Hirshfeld surface analysis of 4-[3-(4-hydroxy-phenyl)-4,5-dihydro-1-pyrazol-5-yl]-2-methoxy-phenol monohydrate. **2019**, 75, 1590-1594
- 542 Crystal structure, DFT and Hirshfeld surface analysis of 2-amino-4-(2-chloro-phenyl)-7-hydroxy-4-benzo[1,2]pyran-3-carbonitrile. **2019**, 75, 1638-1642
- 541 Crystal structure, Hirshfeld surface analysis and inter-action energy and DFT studies of methyl 4-[3,6-bis-(pyridin-2-yl)pyridazin-4-yl]benzoate. **2019**, 75, 1672-1678
- 540 Crystal structure and Hirshfeld surface analysis of 2-(4-nitro-phenyl)-2-oxoethyl 2-chloro-benzoate. **2019**, 75, 1792-1796
- 539 Synthesis and crystal structure of (-)-1,2-bis-[2-(methyl-sulfanyl)phenyl]diazene. **2019**, 75, 1808-1811
- 538 Crystal structures of the two isomeric hydrogen-bonded cocrystals 2-chloro-4-nitro-benzoic acid-5-nitro-quinoline (1/1) and 5-chloro-2-nitro-benzoic acid-5-nitro-quinoline (1/1). **2019**, 75, 1694-1699 2
- 537 Crystal structure, Hirshfeld surface analysis and inter-action energy and DFT studies of (2-(4-benzyl-2-(2,4-dichlorobenzylidene)-2,1,4-benzothiazin-3(4H)-one. **2019**, 75, 1650-1656 3
- 536 Crystal structure and Hirshfeld surface analysis of (2,2')-1,1'-[seleno-bis-(4,1-phenylene)]bis-[3-(4-chlorophenyl)prop-2-en-1-one]. **2019**, 75, 1724-1728 1
- 535 Synthesis, crystal structure and Hirshfeld surface analysis of diethyl 2,6-dimethyl-4-(thiophen-3-yl)-1,4-dihydropyridine-3,5-dicarboxylate. **2019**, 75, 1861-1865
- 534 Crystal structure, Hirshfeld surface analysis and inter-action energy and DFT studies of 1-methyl-3-(prop-2-yn-1-yl)-2,3-dihydro-1,1,3-benzodiazol-2-one. **2019**, 75, 1940-1946
- 533 The crystal structure of the triclinic polymorph of 1,4-bis-([2,2':6',2''-terpyridin]-4'-yl)benzene. **2019**, 75, 1947-1951
- 532 Crystal structure of 4-chloro-2-nitro-benzoic acid with 4-hydroxy-quinoline: a disordered structure over two states of 4-chloro-2-nitro-benzoic acid-quinolin-4(1H)-one (1/1) and 4-hydroxy-quinolinium 4-chloro-2-nitro-benzoate. **2019**, 75, 1853-1856 2
- 531 Crystal structure and Hirshfeld surface analysis of poly[tris-(benzene-1,4-dicarboxylato)tetra-kis-(dimethylformamide)trinickel(II)]: a two-dimensional coordination network. **2019**, 75, 1839-1843
- 530 Hirshfeld surface and theoretical studies of 2,2,2-trichloro-N,N-bis(2-(2,2,2-trichloroacetamido)phenyl)acetamide compound. **2019**, 10, 323-335
- 529 Crystal structure and Hirshfeld surface analysis of 1,2,4-triazolium hydrogen oxalate. **2020**, 76, 137-140
- 528 Crystal structure, characterization and Hirshfeld analysis of bis-((-)-1-[(2,4,6-tribromophenyl)diazonyl]naphthalen-2-olato)copper(II) dimethyl sulfoxide monosolvate. **2020**, 76, 382-386
- 527 The crystal structures and Hirshfeld surface analyses of a cadmium(II) and a zinc(II) mononuclear complex of the new tetrakis-substituted pyrazine ligand ;',',',''-[pyrazine-2,3,5,6-tetra-yltetra-kis-(methyl-ene)]tetra-kis-(methyl-aniline). **2020**, 76, 410-416
- 526 Crystal structure and Hirshfeld surface analysis of 3,6-bis-(pyrimidin-2-yl)-1,4-dihydro-1,2,4,5-tetrazine dihydrate. **2020**, 76, 473-476

- 525 Crystal structure and Hirshfeld surface analysis of 3,4-di-hydro-2-anthra[1,2-][1,4]dioxepine-8,13-dione. **2020**, 76, 576-580
- 524 Crystal structure, Hirshfeld surface analysis and inter-action energy and DFT studies of 2-(2,3-di-hydro-1-perimidin-2-yl)-6-meth-oxy-phenol. **2020**, 76, 605-610
- 523 Crystal structure, Hirshfeld surface analysis and DFT studies of 2-(2,3-di-hydro-1-perimidin-2-yl)phenol. **2020**, 76, 798-802
- 522 The crystal structure and Hirshfeld surface analysis of 1-(2,5-di-meth-oxy-phen-yl)-2,2,6,6-tetra-methyl-piperidine. **2020**, 76, 794-797
- 521 Crystal structure, Hirshfeld surface analysis and inter-action energy, DFT and anti-bacterial activity studies of ()-4-hexyl-2-(4-methyl-benzyl-idene)-2-benzo[[1,4]thia-zin-3(4)-one. **2020**, 76, 889-895
- 520 Stereochemistry of the methyl-idene-bridged quinazoline-iso-quinoline alkaloid 3-[[6,7-dimeth-oxy-1-(4-nitro-phen-yl)-1,2,3,4-tetra-hydro-isoquinolin-2-yl]methyl-idene]-1,2,3,9-tetra-hydro-pyrrolo-[2, methanol monosolvate. **2020**, 76, 914-919
- 519 Crystal structure and Hirshfeld surface analysis of 4-{2,2-di-chloro-1-[(0)-(4-chloro-phen-yl)diazen-yl]ethen-yl}-,di-methyl-aniline. **2020**, 76, 1033-1037
- 518 Crystal structures and Hirshfeld surface analyses of 6,8-dimeth-oxy-3-methyl-1-isochromen-1-one and 5-bromo-6,8-dimeth-oxy-3-methyl-1-isochromen-1-one chloro-form monosolvate. **2020**, 76, 1107-1112
- 517 Crystal structure and Hirshfeld surface analysis of 1-methyl-4-(2-methyl-10-benzo[thieno[2,3-][1,4]diazepin-4-yl)piperazin-1-ium 2,5-di-hydroxy-benzoate propan-2-ol monosolvate. **2020**, 76, 1168-1172
- 516 The crystal structures, Hirshfeld surface analyses and energy frameworks of two hexa-thia-pyrazino-phane regioisomers; 2,5,8,11,14,17-hexa-thia-[9.9](2,6,3,5)-pyrazino-phane and 2,5,8,11,14,17-hexa-thia-[9.9](2,5,3,6)-pyrazino-phane. **2020**, 76, 977-983 1
- 515 Crystal structure and Hirshfeld surface analysis of 1-(2-fluoro-phen-yl)-1-tetra-zole-5(4)-thione. **2020**, 76, 1007-1011 1
- 514 Crystal structure and Hirshfeld surface analysis of 4-{2,2-di-chloro-1-[(0)-2-(4-methyl-phen-yl)diazen-1-yl]ethen-yl}-,di-methyl-aniline. **2020**, 76, 1122-1125 0
- 513 Crystal structure, Hirshfeld surface analysis and DFT studies of ()-4-methyl-2-[[4-methyl-phen-yl]imino]-meth-yl}phenol. **2020**, 76, 1075-1079
- 512 The crystal structure, Hirshfeld surface analysis and energy frameworks of 2-[2-(meth-oxy-carbon-yl)-3,6-bis-(meth-oxy-meth-oxy)phen-yl]acetic acid. **2020**, 76, 1101-1106
- 511 Crystal structure, Hirshfeld surface analysis and DFT studies of 4-methyl-2-[[4-(tri-fluoro-meth-yl)phen-yl]imino]-meth-yl}phenol. **2020**, 76, 1325-1330 1
- 510 Theoretical studies on the role of each component in benzotrifuroxan/2,4,6-trinitrotoluene cocrystal. **2020**, 753, 137608 2
- 509 Crystal structures of [(,-di-methyl-amino)-meth-yl]ferrocene and (, )-bis-{2-[(di-methyl-amino)-meth-yl]ferrocen-yl}di-methyl-silane. **2020**, 76, 1437-1441 1
- 508 Synthesis, Structural Characterization and Hirshfeld Surface Analysis of Mixed Ligand Copper(II) Complex. **2020**, 28, 100374 0

507	Crystal structure, Hirshfeld surface analysis and spectroscopic characterization of the di-enol tautomeric form of the compound 3,3'-[(2-sulfanylidene-1,3-dithiole-4,5-diyl)bis(sulfane-diyl)]bis(pentane-2,4-dione). <b>2020</b> , 76, 1427-1432	1
506	Synthesis, crystal structure, potential drug properties for Coronavirus of Co(II) and Zn(II) 2-chlorobenzoate with 3-cyanopyridine complexes. <b>2021</b> , 1250, 131825	0
505	Synthesis, structural, characterization and Hirshfeld analysis of a bis-selenide and a zinc complex of a new hemilabile ferrocenylbisphosphane, [Fe{CHP(CHCHNMe-o)}]. <b>2021</b> , 77, 725-733	1
504	Molecular, Supramolecular Structures Combined with Hirshfeld and DFT Studies of Centrosymmetric M(II)-azido {M=Ni(II), Fe(II) or Zn(II)} Complexes of 4-Benzoylpyridine. <b>2021</b> , 13, 2026	2
503	Synthesis, crystal structure, Hirshfeld surface analysis and theoretical investigation of polynuclear coordination polymers of cobalt and manganese complexes with nitrobenzene and pyrazine. <b>2021</b> , 1250, 131851	7
502	New Bis-Pyrazole-Bis-Acetate Based Coordination Complexes: Influence of Counter-Anions and Metal Ions on the Supramolecular Structures. <b>2021</b> , 13, 288	1
501	The Bonding Interactions in Fluorinated Vinylogous Amides: A CF <sub>3</sub> -Substituted Carbonyl- $\beta$ -Aminoone as a Case Study. <b>2021</b> , 56, 2000162	
500	Hirshfeld Surface Analysis and Interaction Energy Calculations of Bis(4-chlorophenylacetate)bis(pyridine-4-carboxamide)Zinc(II).	
499	Comparative Study of Chalcones and Their Potential as Additives for Biofuels. <b>2021</b> , 35, 552-560	3
498	Crystal growth, spectroscopic and theoretical investigation of nonlinear optical 2-bromo-4-nitroaniline single crystals for NLO and optoelectronic applications. <b>2022</b> , 1250, 131725	1
497	Crystal structure and Hirshfeld surface analysis of dl-methionine polymorphs (I and II) <b>2022</b> , 1250, 131721	1
496	Supramolecular architectures of mononuclear nickel(II) and homobinuclear copper(II) complexes with the 5,5'-dimethyl-2,2'-bipyridine ligand: Syntheses, crystal structures and Hirshfeld surface analyses. <b>2022</b> , 1250, 131728	0
495	Solid-State NMR, X-Ray Diffraction, and Theoretical Studies of Neutral Mononuclear Molecular Bis(triphenylphosphine)silver(I) Mono-Carboxylate and -Nitrate Systems. <b>2020</b> , 73, 556	
494	Structural and DFT Study of 1-(3-Amino-1,4-dioxo-1,4-dihydronaphthalen-2-yl)-3,4-dichloro-1H-pyrrole-2,5-dione: Hypothesis for the Ring Closure. <b>2020</b> , 100, 1426	
493	Crystal structures and Hirshfeld surface analysis of -bis-(thio-cyanato)-bis-{2,4,6-trimethyl-[(pyridin-2-yl)methyl-idene]aniline-} manganese(II) and -bis-(thio-cyanato)-bis-{2,4,6-trimethyl-[(pyridin-2-yl)methyl-idene]aniline-} nickel(II). <b>2020</b> , 76, 288-293	
492	Crystal structure, Hirshfeld surface analysis, inter-action energy and DFT studies of (2)-2-(2,4-di-chloro-benzyl-idene)-4-nonyl-3,4-di-hydro-2-1,4-benzo-thia-zin-3-one. <b>2020</b> , 76, 281-287	1
491	Crystal structure and Hirshfeld surface analysis of 4-[(anthracen-9-yl)methyl]amino-benzoic acid. <b>2020</b> , 76, 62-65	1
490	Structural characterization and Hirshfeld surface analysis of 2-iodo-4-(penta-fluoro-sulfan-yl)benzo-nitrile. <b>2020</b> , 76, 231-234	1

- 489 Crystal structure and Hirshfeld surface analysis of 4-allyl-2-methoxy-6-nitro-phenol. **2020**, 76, 461-465
- 488 Syntheses and crystal structures of a new pyrazine dicarboxamide ligand, ,  
-bis-(quinolin-8-yl)pyrazine-2,3-dicarboxamide, and of a copper perchlorate binuclear complex. **2020**  
, 76, 332-338
- 487 Crystal structures and Hirshfeld surface analyses of two new tetra-kis-substituted pyrazines and a  
degradation product. **2020**, 76, 404-409 1
- 486 Crystal structure, Hirshfeld surface analysis and DFT studies of  
1-[2,6-diphenyl-3-(propan-2-yl)piperidin-1-yl]ethan-1-one. **2020**, 76, 377-381
- 485 Interactions in flavanone and chalcone derivatives: Hirshfeld surface analysis, energy frameworks  
and global reactivity descriptors. **2020**, 76, 212-224 0
- 484 Crystal structure, Hirshfeld surface analysis and inter-action energy and DFT studies of  
()-10-propargyl-pyrrolo-[2,1-][1,4]benzodiazepine-5,11-dione. **2020**, 76, 467-472
- 483 Silver(I) nitrate two-dimensional coordination polymers of two new pyrazine-thio-phane ligands:  
5,7-di-hydro-1,3-dithieno[3,4:3',4'-]pyrazine and  
3,4,8,10,11,13-hexa-hydro-1,6-bis-([1,4]di-thio-cino)[6,7:6',7'-]pyrazine. **2020**, 76, 539-546 3
- 482 Crystal structure of (4-chloro-phen-yl)(4-methyl-piperidin-1-yl)methanone. **2020**, 76, 534-538 0
- 481 Crystal structure and Hirshfeld surface analysis of 4-[(anthracen-9-yl)meth-yl]amino}-benzoic acid  
di-methyl-formamide monosolvate. **2020**, 76, 728-731
- 480 Crystal structure, Hirshfeld surface analysis and inter-action energy, DFT and anti-bacterial activity  
studies of ethyl  
2-[(2)-2-(2-chloro-benzyl-idene)-3-oxo-3,4-di-hydro-2-1,4-benzo-thia-zin-4-yl]acetate. **2020**, 76, 629-636
- 479 Crystal structure, Hirshfeld surface analysis and DFT studies of  
6-bromo-3-(12-bromo-dodec-yl)-2-(4-nitro-phen-yl)-4-imidazo[4,5-]pyridine. **2020**, 76, 677-682 2
- 478 Assembly of two pharmaceutical salts of sparfloxacin with pyrocatechuic acid: Enhancing in vitro  
antibacterial activity of sparfloxacin by improving the solubility and permeability. **2021**, 1250, 131894 0
- 477 New binuclear mercury complex: Synthesis, supramolecular structure, physico-chemical  
characterizations and antibacterial activity. **2021**, 1250, 131829
- 476 Dihydrofolate Reductase Inhibitors: The Pharmacophore as a Guide for Co-Crystal Screening. **2021**,  
26, 1
- 475 Influence of Hydroxyl Group Position and Substitution Pattern of Hydroxybenzoic Acid on the  
Formation of Molecular Salts with the Antifolate Pyrimethamine. 2
- 474 Synthesis and structural study of five new phosphoric triamides: interplay between classical and  
non-classical intermolecular interactions. **2021**, 0
- 473 Understanding Hygroscopicity of Theophylline a Novel Cocrystal Polymorph: A Charge Density  
Study. **2021**, 125, 9736-9756 1
- 472 Crystal structure and Hirshfeld surface analysis of 2,6-di-iodo-4-nitro-toluene and  
2,4,6-tri-bromo-toluene. **2020**, 76, 1391-1397

- 471 Crystal structure, Hirshfeld surface analysis and DFT studies of 2-[(2-hydroxy-5-methyl-benzyl-iden)amino]-benzo-nitrile. **2020**, 76, 1195-1200 1
- 470 Crystal structure of 1-ferrocenyl-2-(4-nitro-phen-yl)ethyne. **2020**, 76, 1403-1406 1
- 469 Crystal structure, Hirshfeld surface analysis and DFT study of 6-bromo-3-(5-bromo-hex-yl)-2-[4-(di-methyl-amino)-phen-yl]-3-imidazo[4,5-]pyridine. **2020**, 76, 1234-1238 1
- 468 Crystal structure, Hirshfeld surface analysis and DFT studies of (O-4-methyl-2-[[2-methyl-3-nitro-phen-yl]imino]-meth-yl]phenol. **2020**, 76, 1551-1556 0
- 467 On the Hirshfeld surface for copper(II) atoms in different coordination environments. **2020**, 53, 1321-1333 0
- 466 Synthesis, crystal structure and Hirshfeld surface analysis of bis-{2-[(pyridin-2-yl)amino]-pyridinium} tetra-cyano-nickelate(II). **2020**, 76, 1794-1798
- 465 Crystal Structure, Hirshfeld Surface Analysis, and Absorption Spectra of a New Polymorph of Highly Symmetric Tetraphenylporphyrinato Zn(II), ZnTPP. **2020**, 65, 933-946
- 464 The superiority of the classical synthesis compared to the hydrothermal synthesis upon the structural, optical absorption and fluorescent properties of new Cd(II) 3-fluorobenzoate complexes with Pyridine-3-carboxamide/Pyridine-3-carboxylate. **2020**, 509, 119694 0
- 463 On the importance of intermolecular interactions of 3-(2,3-dihydroxy-isopentyl)-4-hydroxyacetophenone: Crystal structure, spectroscopic and hirshfeld surface analysis. **2020**, 1217, 128393 1
- 462 Neutral nickel(II) complex bearing hemilabile N,S-donor ligands: Structural, Hirshfeld surfaces and DFT studies. **2020**, 709, 98-110 2
- 461 Crystal structures of four isomeric hydrogen-bonded co-crystals of 6-methyl-quinoline with 2-chloro-4-nitro-benzoic acid, 2-chloro-5-nitro-benzoic acid, 3-chloro-2-nitro-benzoic acid and 4-chloro-2-nitro-benzoic acid. **2020**, 76, 1701-1707 2
- 460 Oxaphosphacyclophanes Constructed from a Bis(triphenylphosphine oxide) Moiety Linked by Dioxyalkyl Chains: Synthesis and Crystal Structures. **2020**, 5, 23621-23630
- 459 Crystal structure and Hirshfeld analysis of di-n-butyl 2,2'-[(ethyl-aza-nedi-yl)bis-(methyl-ene)]bis-(1-pyrrole-1-carboxyl-ate). **2020**, 76, 1827-1831
- 458 Ethyl 5-methyl-3-[11-(pyridin-2-yl)-6,11-di-hydro-6,11-ep-oxy-dibenzo[,oxepin-6-yl]isoxazole-4-carboxylate: a bicyclic acetal from the rearrangement of an anthracenyl isoxazole. **2020**, 76, 1818-1822
- 457 Hexahalorhenate(IV) salts of protonated ciprofloxacin: antibiotic-based single-ion magnets. 3
- 456 A comparative study of noncovalent interactions in various Ni-compounds containing nitrogen heteroaromatic ligands and pseudohalides: A combined experimental and theoretical studies. **2022**, 531, 120702
- 455 Synthesis, crystal structure and Hirshfeld surface analysis of the binuclear Cu(II) complex with 4-nitrobenzoic acid and triethanolamine. **2022**, 37, 100802 0
- 454 Revealing the dissolution behavior of trans-p-methoxycinnamic acid in 12 organic solvents by parametric model and molecular simulation. **2022**, 166, 106683 1

- 453 Phosphorus-nitrogen compounds. Part 58. Syntheses, structural characterizations and biological activities of 4-fluorobenzyl-spiro(N/O)cyclotriphosphazene derivatives. **2021**, 1-21 3
- 452 New preparation protocols for coumarin-thiosemicarbazone hybrids: solid state characterization, and in silico/NMR studies of the Z/E isomerization equilibria in solution. **2021**, 131980 0
- 451 Single crystal X-ray diffraction, Hirshfeld surface analysis and DFT studies of Bis(L-Serinium) oxalate dihydrate (BLSOD). **2021**, 2070, 012099
- 450 Thermo-Induced Single-Crystal-to-Single-Crystal Transformations and Photo-Induced [2+2] Cycloaddition Reactions in Polymorphs of Chalcone-Based Molecular Crystals: Multi-Stimuli Responsive Actuators. **2021**, 2 2
- 449 Self-Assembly of a Lantern-Like Zirconium Metal-Organic Cage Decorated with  $\beta$ -OH Functional Groups for Potential Al<sup>3+</sup> Ion Detection. **2021**, 21, 6642-6647 1
- 448 Crystal structure and optical property of a supramolecular bromotellurate salt templated with 4 (Ethylammoniummethyl)pyridinium. **2021**, 1251, 131994 0
- 447 Hirshfeld Surface Method and Its Application in Energetic Crystals. **2021**, 21, 6619-6634 3
- 446 Crystal structure, DFT studies, Hirshfeld surface and energy framework analysis of 4-(5-nitro-thiophen-2-yl)-pyrrolo [1, 2-a] quinoxaline: A potential SARS-CoV-2 main protease inhibitor. **2021**, 131932 4
- 445 Supramolecular structure and spectroscopic characterization of new 1,3,5-triaza-2-boracyclohex-3-en derivative formed under mild conditions between 2-imino-4-thiobiuret and boric acid. **2021**, 131968 0
- 444 The Effect of the Side Chain on Gelation Properties of Bile Acid Alkyl Amides. **2021**, 10, 1150-1157 0
- 443 Crystal structure, quantum computational, molecular docking and in vitro anti-proliferative investigations of 1H-imidazole-2-thione analogues derivative. **2021**, 1250, 131833 0
- 442 2,4-bis(bromomethyl)-1,3,5-trimethylbenzene with 2-mercaptopyridine based derivative: Synthesis, crystal structure, in vitro anticancer activity, DFT, Hirshfeld surface analysis, antioxidant, DNA binding and molecular docking studies. **2021**, 1251, 131981 0
- 441 TNB/TNCB cocrystal  $\beta$  an insensitive energetic cocrystal with low melting point. 1-14 1
- 440 Synthesis and characterization of a new zero-dimensional organic-inorganic hybrid material based on antimony. **2021**, 1251, 132012 0
- 439 A second solvatomorph of poly[[[E]-(1,3,5-oxadiazinane-3,5-di-yl)bis-(carbamoyl-methano-ato)]nickel(II)dipotassium]: crystal structure, Hirshfeld surface analysis and semi-empirical geometry optimization.. **2021**, 77, 1289-1295
- 438 Series of Ln-metal organic frameworks: Photocatalytic performance and Hirshfeld surface analyses. **2021**, 131956 3
- 437 Molecular salts of the isoniazid derivatives. Expanding the scope of sulfonate-pyridinium synthon to design materials. **2021**, 307, 122762 1
- 436 Synthesis, structural characterization, Hirshfeld surface analysis and anti-corrosion on mild steel in 1M HCl of ethyl 2-(3-methyl-2-oxo-1,2-dihydroquinoxaline-1-yl)acetate. **2021**, 1251, 132047 0



- 435 Synthesis, structure and Hirshfeld surface analysis of a series of novel low melting salts without alkyl groups. **2021**, 23, 8150-8158
- 434 Pseudotetrahedral Zn(II)-( or )-dihalogen-salicylaldiminato complexes with E or E chirality induction at-metal.. **2022**, 0
- 433 Crystal structure, vibrational spectra, optical properties and thermal behavior of the 1D perovskite (2-amino-4-methylpyridinium)trichlorocadmate(II) (C<sub>6</sub>H<sub>9</sub>N<sub>2</sub>)<sub>1</sub>[CdCl<sub>3</sub>]. 1-13 2
- 432 (E)-5-Fenil-N-(2-tiyenilmetilen)-1,3,4-tiyadiazol-2-aminin Hirshfeld Yzey Analizi ve Teorik Hesaplamalar-. 0
- 431 Crystal structure, surface analysis, and computational investigations of 1-(4-chloro-3-nitrophenyl)-6,7-dihydro-1H-benzo[d][1,2,3]triazol-4(5H)-one as potential acceptor molecule for photovoltaics applications. **2022**, 1254, 132349 1
- 430 An insight into triel bonds in O,O'-diarylphosphorodithioates of thallium(I): experimental and theoretical investigations. **2022**, 46, 832-843 2
- 429 Cu(II) and Zn(II) complexes incorporated with active analogue fragments molecule of the aristolochic acid: Crystal structure and biological activity. **2022**, 1252, 132172 3
- 428 In vitro biological activity of copper(II) complexes with NSAIDs and nicotinamide: Characterization, DNA- and BSA-interaction study and anticancer activity.. **2021**, 228, 111696 1
- 427 Crystal structure elucidation and DFT studies of imidazopyridine-pyrazoline derivative. **2022**, 1251, 132063 1
- 426 Spodium bonds and metalhalogen-halogenmetal interactions in propagation of monomeric units to dimeric or polymeric architectures. **2022**, 1252, 132144 1
- 425 Structural insights and antioxidant analysis of a tri-methoxy chalcone with potential as a diesel-biodiesel blend additive. **2022**, 227, 107122 4
- 424 Intermolecular (Isocyano group)-PtII interactions involving coordinated isocyanides in cyclometalated PtII complexes. **2022**, 1253, 132230 2
- 423 The synthesis, structure, and spectral properties of antimony(III) phthalocyanine obtained under iodine vapor atmosphere: (SbIII Pc)(I<sub>3</sub>) · (I<sub>2</sub>). **2022**, 532, 120758 0
- 422 Polymorphism and solid state peculiarities in imidazo[1,5-a]pyridine core deriving compounds: An analysis of energetic and structural driving forces. **2022**, 1253, 132175 2
- 421 Crystal structure elucidation, Hirshfeld surface analysis, and DFT studies of a N-benzyl-3-phenylquinoxalin-2-amine. **2022**, 1253, 132271 1
- 420 Oxaphosphacyclophanes Constructed from a Bis(triphenylphosphine oxide) Moiety Linked by Dioxyalkyl Chains: Synthesis and Crystal Structures. **2020**, 5, 23621-23630 0
- 419 Crystal structure and Hirshfeld analysis of di-tert-butyl 2,2'-[(ethylazanediy)bis(methylene)]bis(1H-pyrrole-1-carboxylate). **2020**, 76, 1827-1831
- 418 Ethyl 5-methyl-3-[11-(pyridin-2-yl)-6,11-dihydro-6,11-epoxydibenzo[b,e]oxepin-6-yl]isoxazole-4-carboxylate: a bicyclic acetal from the rearrangement of an anthracenyl isoxazole. **2020**, 76, 1818-1822 0



- 399 Synthesis, crystal structure and Hirshfeld surface analysis of dimethyl 3-(3-bromo-phen-yl)-6-methyl-7-oxo-3,5,6,7-tetra-hydro-pyrazolo-[1,2-]pyrazole-1,2-di-carboxyl-ate.. **2022**, 78, 125-129
- 398 Architectural View of Flexible Aliphatic  $\text{DH}$  Group Coordinated Hemi-Directed Pb(II)-Salen Coordination Polymer: Synthesis, Crystal Structure, Spectroscopic Insights, Supramolecular Topographies, and DFT Perspective. **2022**, 32, 1159 2
- 397 Growth, crystal structure, Hirshfeld surface and vibrational properties of a new supramolecular hybrid material:  $(\text{C}_4\text{H}_7\text{N}_2)_2\text{TeBr}_6$ . 1 0
- 396 Shedding Light on the Synthesis, Crystal Structure, Characterization, and Computational Study of Optoelectronic Properties and Bioactivity of Imine derivatives.. **2022**, 7, 5217-5230 4
- 395 Synthesis, crystal structure, Hirshfeld surface analysis and molecular docking analysis of new cadmium(II) iodide complex with the pyridine, 4-(1,1-dimethylethyl). 1-23 0
- 394 Positional effects of a pyridyl group in Zn(II) coordination polymers on the selective dye adsorption properties. **2022**, 214, 115646 1
- 393 Monomeric octahedral bismuth(III) benzaldehyde-N1-alkyl thiosemicarbazones: Synthesis, characterization and biological properties. **2022**, 215, 115683 2
- 392 Synthesis, crystal structure and molecular docking studies of novel Schiff base ligand 9-(((3-ethyl-5-mercapto/thio-4H-1,2,4-triazole-4-yl)imino)methyl)-anthracene and its complexes with Ni(II), Cu(II), Zn(II) and Cd(II): Comparative spectral, thermo-kinetics, radical scavenging and antimicrobial studies. **2022**, 38, 188833 1
- 391 Crystal engineering with energetic picric acid halogen-based salts: Promising properties of a new family of insensitive materials. **2022**, 1254, 132381 1
- 390 Counteranion-solvent-dependent construction of two octahedral homopolynuclear Ni(II) complexes with a symmetrical multi-halogen-substituted bis(salamo)-based ligand. **2022**, 534, 120815 3
- 389 Synthesis, characterization, crystal structure determination, computational modelling and biological studies of a new tetrakis-(2-hydroxy-5-methylphenyl)(1H-pyrazol-4-yl)methanonezinc(II) complex. **2022**, 1255, 132377 1
- 388 A bowl-shaped phenoxido-bridged binuclear zinc complex: Experimental and theoretical studies. **2022**, 534, 120807 0
- 387 Expanding the Scope of Hydroxyl-pyridine Supramolecular Synthons to Design Molecular Solids. 1
- 386 Synthesis, molecular and supramolecular structure aspects and biological evaluations of a novel  $[\text{Ag}_2(\text{phthalazine})(\text{NO}_3)_2]_n$  3D coordination polymer. **2022**, 132592 1
- 385 Efficient Consecutive Synthesis of Ethyl-2-(4-Aminophenoxy) Acetate, a Precursor for Dual GK and PPAR $\alpha$  Activators, X-ray Structure, Hirshfeld Analysis, and DFT Studies. **2022**, 12, 227
- 384 Synthesis, structural characterization, antibacterial activity, DFT computational studies and thermal analysis of two new thiocyanate compounds based on 1-phenylpiperazine. **2022**, 1257, 132620 0
- 383 Transport in Twisted Crystalline Charge Transfer Complexes. 3
- 382 Experimental and computational studies on copper(II) Schiff base complex derived from 4-acetyl-3-methyl-1-phenyl-2-pyrazolin-5-one. **2022**, 132626 2

- 381 Molecular Packing of Phenoxazine: A Combined Single-Crystal/Crystal Structure Prediction Study. 0
- 380 New gem-dichlorocyclopropane-pyrazole hybrids with monoterpene skeleton: Synthesis, crystal structure, cytotoxic evaluation, molecular dynamics and theoretical study. **2022**, 1256, 132573
- 379 Synthesis, structural, computational, and antiproliferative activity studies of new steroidal tetrazole derivatives. **2022**, 1256, 132577 0
- 378 Experimental and computational tuning of metalla-N-heterocyclic carbenes at palladium(II) and platinum(II) centers.. **2022**, 1
- 377 Experimental and theoretical insights into the formation of weak hydrogen bonds and H<sup>+</sup>H bonding interactions in the solid-state structure of two eucalyptol derivatives. **2022**, 46, 5690-5704 0
- 376 Analysis of the solvent effects on the crystal growth of peripherally chlorinated boron subphthalocyanines.
- 375 Structural Investigations, Hirshfeld Surface, Vibrational and Nmr Spectroscopies Analysis of a New Hybrid Complexes: (C<sub>6</sub>H<sub>10</sub>N<sub>2</sub>).Cl<sub>2</sub> (I) and [C<sub>6</sub>H<sub>10</sub>N<sub>2</sub>]<sub>2</sub>ZnCl<sub>4</sub> (II).
- 374 Two novel TNB energetic cocrystals with low melting point: a potential strategy to construct melt cast explosive carriers. 2
- 373 Effect of substituents in novel bioactive tavorole derivatives on intermolecular interactions hierarchy. 1
- 372 Static discrete disorder in the crystal structure of iododiflunisal: on the importance of hydrogen bond, halogen bond and π-stacking interactions. 2
- 371 Hydrogen Bond and π-stacking Interaction: Stabilization Mechanism of Two Metal -N -Containing Energetic Materials.. **2022**, 7, 6627-6639
- 370 Multifunctional Silver(I) Complexes with Metronidazole Drug Reveal Antimicrobial Properties and Antitumor Activity against Human Hepatoma and Colorectal Adenocarcinoma Cells.. **2022**, 14, 1
- 369 Crystal structures and Hirshfeld surface analysis of 5-amino-1-(4-methoxyphenyl)pyrazole-4-carboxylic acid and 5-amino-3-(4-methoxyphenyl)isoxazole.. **2022**, 78, 336-339
- 368 Crystal structures of three thalolactic acids: hydrogen bonding resulting in differing Z'.. **2022**, 78, 257-264 0
- 367 Crystal structure and Hirshfeld surface analysis of tris-(acetohydrazide-κ)(nitrate-κ)(nitrate-κ)terbium(III) nitrate.. **2022**, 78, 354-358
- 366 Giant Supramolecular Synthons via Cyclic Halogen...Halogen Contacts in Substituted o-Xylenes. **2022**, 22, 2318-2327 4
- 365 Experimental and theoretical study of novel amino-functionalized P(V) coordination compounds suggested as inhibitor of M of SARS-COV-2 by molecular docking study.. **2022**, 36, e6636 0
- 364 Synthesis, crystal structure, Hirshfeld surface investigation and comparative DFT studies of ethyl 2-[2-(2-nitrobenzylidene)hydrazinyl]thiazole-4-carboxylate.. **2022**, 16, 18 3

- 363 Synthesis, Structural Investigation, Hirshfeld Surface Analysis, and Biological Evaluation of - (3-Cyanothiophen-2-yl)-2-(thiophen-2-yl)acetamide.. **2022**, 7, 11320-11329 0
- 362 Prediction of the crystal structure and properties of energetic LLM -105:oxidant cocrystals: A theoretical study.
- 361 Supramolecular Self-Assembly Built by Hydrogen, Stacking and Br<sup>δ+</sup>Br<sup>δ-</sup> Interactions in 4-((4-Bromobenzyl)Selenyl)Aniline: Structure, Hirshfeld Surface Analysis, 3D Energy Framework Approach and Global Reactivity Descriptors. 1 0
- 360 Linear Supramolecular Polymer Driven by Br<sup>δ+</sup>Br<sup>δ-</sup> and Br<sup>δ+</sup>H Non-bonding Interactions Based on Inclusion-Complex of Octabromo-Functionalized Pillar[5]arene. 1 1
- 359 Crystal structure, Hirshfeld surface analysis, inter-action energy and DFT calculations and energy frameworks of methyl 6-chloro-1-methyl-2-oxo-1,2-di-hydro-quinoline-4-carboxyl-ate.. **2022**, 78, 425-432 0
- 358 Synthesis, Structure, and UV-Vis Characterization of Antimony(III) Phthalocyanine: [(SbPc)(SbI)(SbBr)].. **2022**, 27, 0
- 357 Supramolecular Arrangement Built from Zinc and Cadmium Complexes with 4-(4-Substituted)-2,2':6,2'-Terpyridine: Crystallographic Investigation, Luminescence and Thermal Properties. 1 0
- 356 Robustness of hydrogen bonding in the construction of supramolecular architectures in protonated perchlorate salts.. **2022**, 28, 74
- 355 Crystal structure and Hirshfeld surface analysis of ()-1-[2,2-di-bromo-1-(2-nitro-phen-yl)ethen-yl]-2-(4-fluoro-phen-yl)diazene.. **2022**, 78, 404-408 1
- 354 Crystal structure and Hirshfeld surface analysis of 2-(2-hydroxy-phen-yl)quinoline-6-sulfonamide.. **2022**, 78, 409-413
- 353 Synthesis, Crystal Structures and Hirshfeld Surface Analysis of Bis[di(2-methoxyphenyl)phosphoroselenoyl]-2,4-cyclopentadien-1-yl]iron(II) and Ruthenium(II)π-arene Complex of Bis-[di(2-allylphenyl)phosphonite]-2,4-cyclopentadien-1-yl]iron(II). 1
- 352 Crystal Structure Characterization, Hirshfeld Surface Analysis, and Non-covalent Interactions of 2,5-Bis(4-chlorophenyl)-1,3,4-Oxadiazole. 1 0
- 351 Synthesis of Crystalline Fluoro-Functionalized Imines, Single Crystal Investigation, Hirshfeld Surface Analysis, and Theoretical Exploration.. **2022**, 7, 9867-9878 6
- 350 Synthesis, Molecular Structure, Thermal and Spectroscopic Analysis of a Novel Bromochalcone Derivative with Larvicidal Activity. **2022**, 12, 440 2
- 349 Insights Into the Properties of Amygdalin Solvatomorphs: X-ray Structures, Intermolecular Interactions, and Transformations.. **2022**, 7, 8906-8918 1
- 348 Design Strategy of Highly Efficient Nonlinear Optical Orange-Colored Crystals with Two Electron-Withdrawing Groups. 2100350 1
- 347 Dissolution behavior, thermodynamic and kinetic analysis of malonamide by experimental measurement and molecular simulation. **2022**,
- 346 Combined Experimental and Theoretical Investigations on 9-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,9-dihydro-6H-purin-6-one 4-nitrophenol (IPNP) Molecule. **2022**, 133020

- 345 Remarkable Nonlinear Properties of a Novel Quinolidone Derivative: Joint Synthesis and Molecular Modeling.. **2022**, 27, 0
- 344 Synthesis, crystal structure, computational, and molecular docking studies of bis {1,1'-[1,3,5-Trimethyl-1,3-phenylenebis(methylene)]di-1H-piperidinium}tetrabromide tri hydrate. 1-18
- 343 Aggregation-induced dual phosphorescence from (o-bromophenyl)-bis(2,6-dimethylphenyl)borane at room temperature.. **2022**, 1
- 342 Iron(II), cobalt(II), and nickel(II) complexes with 1,10-phenanthroline and 2,2'-bipyridyl and the macropolyhedral borane cluster [trans-B20H18]2- as counterion. **2022**, 217, 115740 0
- 341 Acesulfame based Co(II) complex: Synthesis, structural investigations, solvatochromism, Hirshfeld surface analysis and molecular docking studies. **2022**, 218, 115762 5
- 340 A novel 3D Ag (I) metal-organic coordination polymer (Ag-MOCP): Crystallography, Hirshfeld surface analysis, antibacterial effect and molecular docking studies. **2022**, 310, 123013 1
- 339 Synthesis, structure, NBO, Hirshfeld surface, NMR, HOMO-LUMO, UV, photoluminescence, z scan, vibrational and thermal analysis of piperazinedi-ium tetrakis (2-chloro)-diaqua-dichloro-di-cadmium single crystal. **2022**, 1258, 132685 0
- 338 Remote hydroxyl group induced structural diversities in antimony(III) chalcogenones. **2022**, 219, 115795
- 337 Investigating the synthesis and structure of [2]pseudorotaxanes assembled by crown ether as wheel component and dual-cation axle with phosphonium and ammonium cations. **2022**, 1259, 132721
- 336 New bioactive 1D Ag(I) coordination polymers with pyrazole and triazine ligands; Synthesis, X-ray structure, Hirshfeld analysis and DFT studies. **2022**, 537, 120948 1
- 335 Energy frameworks and Hirshfeld surface analysis of supramolecular features in three new phosphoric triamides: tuning the intermolecular interactions via the substituent effect. **2022**, 1259, 132742 0
- 334 Single crystal structure, thermal stability and theoretical studies of ethyl 4-(4-(dimethylamino)phenyl)-3,6-dimethyl-1-phenyl-1H-pyrazolo[3,4-b]pyridine-5-carboxylate. **2022**, 1260, 132826
- 333 A photo-reversible, sensitive, and selective sensor for copper ions in an aqueous medium. **2022**, 1260, 132807 0
- 332 Importance of non-covalent interactions in a nitrile anion metal-complex based on pyridine ligands: A theoretical and experimental approach. **2022**, 1261, 132885 0
- 331 Synthesis, crystal structure, DFT studies and Hirshfeld surface analysis of Manganese(II) and Cadmium(II) coordination polymers of 2-aminopyridine and dicyanamide. **2022**, 1261, 132956 0
- 330 Crystal structure and photoluminescence properties of a supramolecular hybrid bisulfate and hydrogenphosphate salts. **2022**, 1261, 132816
- 329 Synthesis, Crystal Structure and Hirshfeld Surface Analysis of Ethyl 4-(4-(2-Bromoethyl)-1H-1,2,3-triazol-1-yl)benzoate. **2021**, 66, 977-984
- 328 Crystal structure, Hirshfeld surface, and DFT studies of 4-((pyrrolidin-1-ylsulfonyl)methyl)aniline. **2021**, 12, 419-431

327	Depicting the DNA Binding and Cytotoxicity Studies against Human Colorectal Cancer of Aquabis (1-Formyl-2-Naphtholato-k <sub>2</sub> O,O?) Copper(II): A Biophysical and Molecular Docking Perspective. <b>2022</b> , 12, 15	1
326	Crystal structure, Hirshfeld surface analysis, and DFT studies of N-(2-chlorophenylcarbamoithiyl)cyclohexanecarboxamide. <b>2021</b> , 12, 439-449	0
325	X-ray diffraction and Density Functional Theory based structural analyses of 2-phenyl-4-(prop-2-yn-1-yl)-1,2,4-triazolone. <b>2021</b> , 12, 459-468	
324	Chiral Zn-Based Organic-Inorganic Hybrid Ferroelectrics with Large Polarization and Luminescence. <b>2022</b> , 10, 2101905	5
323	Distinguishment of Weak Interactions of Hydrogen Atoms Bound to Carbon Atoms: X-Ray Crystal Structural and Hirshfeld Surface Analyses of 2-Hydroxy-7-methoxy-3-(2,4,6-trimethylbenzoyl)naphthalene with the 2-Methoxylated Homologue. <b>2021</b> , 10	0
322	Kobalt(II) 4-Floro- ve 4-Bromobenzoat Nikotinamid Komplekslerinin Hirshfeld Yüzey Analizi, Etkilem Enerjisi Hesaplamalar ve Koronavirüs Spike Proteinini ile Etkilemlerinin Moleküler Docking İle İncelenmesi.	
321	Synthesis, Crystal Structures, and Molecular Properties of Three Nitro-Substituted Chalcones. <b>2021</b> , 11, 1589	2
320	Polymorphism in the 1/1 Pterostilbene/Picolinic Acid Cocrystal.. <b>2022</b> , 22, 590-597	1
319	Exoergic pathways triggered by O/H radicals in different metallic carbohydrazide perchlorates (M = Mn, Fe, Co, Ni, Zn and Cd).. <b>2022</b> ,	0
318	Synthesis, crystal structure, hirshfeld surface analysis, molecular docking and molecular dynamics studies of novel olanzapinium 2,5-dihydroxybenzoate as potential and active antipsychotic compound. <b>2022</b> , 17, 247-273	1
317	Structural, Computational and 3D Interaction Energy Calculations of the Compound 2-chloro-3-(1-naphthyl)-5,5-dimethyl-2-cyclohexenone. <b>2022</b> , 67, 201-208	1
316	Experimental Spectroscopic, Quantum Computational, Hirshfeld Surface, Molecular Docking, and Electronic Excitation Studies on an Antibiotic Agent: SDZ. 1-25	1
315	Synthesis, crystal structure and spectroscopic characterization of new anionic iridium(III) complexes and their interaction with biological targets. <b>2022</b> , 115837	1
314	A Combined Experimental and Theoretical Studies of two new Decavanadate: (C <sub>6</sub> N <sub>2</sub> H <sub>9</sub> ) <sub>4</sub> [H <sub>2</sub> V <sub>10</sub> O <sub>28</sub> ] <sub>4</sub> ·4H <sub>2</sub> O and (C <sub>7</sub> H <sub>9</sub> NF) <sub>4</sub> [H <sub>2</sub> V <sub>10</sub> O <sub>28</sub> ] <sub>4</sub> ·4H <sub>2</sub> O. <b>2022</b> , 133085	
313	Single crystal structure features of a new synthesized heteronuclear Mn/Cu complex, a precursor for heterogeneous catalytic conversion of CO. <b>2022</b> , 133109	
312	Structural, Optical, Spectral, Thermal and Third-order NLO Behaviour of 4-Chlorobenzhydrazide Trichloro Acetate Single Crystal. <b>2022</b> , 52, 1	
311	Structural insights and supramolecular description of Gliclazide and its Impurity F. <b>2022</b> , 1212, 113707	0
310	Synthesis, single-crystal exploration, hirshfeld surface analysis, and DFT investigation of the thiosemicarbazones. <b>2022</b> , 1262, 133088	4

- 309 Preparation, characterization and computational study of mosapride solvates. **2022**, 1262, 133082
- 308 Investigation of solid state architectures in tetrazolyl tryptophol stabilized by crucial aromatic interactions and hydrogen bonding: Experimental and theoretical analysis. **2022**, 1262, 133079 0
- 307 Achieving halogen bonding enhanced ultra-highly efficient AIE and reversible mechanochromism properties of TPE-based luminogens: position of bromine substituents. 2
- 306 Thermosaliency coupled to abrupt spin crossover with dynamic ligand motion in an iron(II) molecular crystal. 2
- 305 Experimental and Hirshfeld Surface Investigations for Unexpected Aminophenazone Cocrystal Formation under Thiourea Reaction Conditions via Possible Enamine Assisted Rearrangement. **2022**, 12, 608 1
- 304 Auophilic Interactions in Cationic Three-Coordinate Gold(I) Bipyridyl/Isocyanide Complex. **2022**, 12, 613 0
- 303 Synthesis, X-ray, characterization and HSA and energy framework analysis of novel pyridine-hydrazone based ligand and its Co(II) complex biological activity prediction and experimental antibacterial properties. 1-20 0
- 302 N-(Sikloheksil(metil)karbamotiyoil)-4-nitrobenzamid Bileşimin Sentezi, Kristal Yapısı, DFT İlgili Analizi ve Hirshfeld Yüzey Analizi. 0
- 301 Preparation, QTAIM and Single-Crystal Exploration of the Primethamine-Based Co-Crystal Salts with Substituted Benzoic Acids. **2022**, 7, 2
- 300 Structure, optical and magnetic properties of the pyridinium cobaltate (C<sub>6</sub>H<sub>9</sub>N<sub>2</sub>)<sub>2</sub>[CoCl<sub>4</sub>]. **2022**, 121003
- 299 Spectroscopic, quantum chemical and molecular docking studies on friedelin, the major triterpenoid isolated from *Garcinia imberti*. **2022**, 1263, 133152 1
- 298 Fluorescent Cu<sup>2+</sup> sensor based on phenanthroline-BODIPY conjugate: A mechanistic study. **2022**, 203, 110343 2
- 297 Effect of alkyl chains on luminescence properties with 3-hydroxy-2-naphthoate esters. **2022**, 1264, 133220 1
- 296 Crystal structure and optoelectronic properties of a supramolecular chlorobismuthate salt templated with 4-pyridiniumthioamide. **2022**, 1263, 133142 0
- 295 Phosphorus-nitrogen compounds. Part 62. Preparation of tetraaminobis(4-fluorobenzyl)spiro(N,N)cyclotriphosphazenes: Chemical, structural characterizations, antimicrobial, antioxidant and DNA-binding activity studies. **2022**, 538, 121001 1
- 294 Synthesis, structural, photo-physical properties and DFT studies of some diarylheptanoids. **2022**, 133254 1
- 293 Synthesis, Crystal Structure, Hirshfeld Surface Analysis and Interaction Energy and Energy Framework Studies of Novel Hydrazone Derivative Containing Barbituric Acid Moiety. 0
- 292 A new strategy to design isostructural salts: the case of the antitumor drug dimethylaminomicheliolide. **2022**, 1262, 133082 0



- 291 Significant photodegradation of carcinogenic organic dyes by 1D supramolecular heteroleptic Cu(II) complex on sunlight irradiation. 1
- 290 Crystalline Derivatives of Dipyrazolo-1,5-diazocine and Dipyrazolopyrimidine: A Case of Unexpected Synthesis and Isostructural Polymorphism. **2022**, 12, 714
- 289 Microwave Assisted Synthesis, Crystal Structure and Hirshfeld Surface Analysis of Some 2-Formimidate-3-carbonitrile Derivatives Bearing 4H-Pyran and Dihydropyridine Moieties. **2022**, 2022, M1364
- 288 X-ray and DFT calculations of novel spiroisoxazolines derivatives. **2022**, 133324 1
- 287 Theoretical Studies on the Role of Guest in  $\beta$ -CL-20/Guest Crystals. **2022**, 27, 3266 0
- 286 Synthesis, X-ray diffraction analysis, quantum chemical studies and  $\beta$ -amylase inhibition of probenecid derived S-alkylphthalimide-oxadiazole-benzenesulfonamide hybrids. **2022**, 37, 1464-1478 4
- 285 Co (II) Complexes Based on the Bis-Pyrazol-S-Triazine Pincer Ligand: Synthesis, X-ray Structure Studies, and Cytotoxic Evaluation. **2022**, 12, 741 1
- 284 Optimized Structure, in Silico interaction and Molecular Docking Analysis of Two Benzimidazole-2-Thione Derivatives. **2022**, 19, 01-16
- 283 Novel copper(II) and nickel(II) coordination complexes of 2,4-pentanedione bis-thiosemicarbazone: Synthesis, structural characterization, computational studies, and magnetic properties. **2022**, 141, 109574 1
- 282 Syntheses, crystal structures, hirshfeld surface analyses and electrochemical etoposide/camptothecin sensor applications of acetaldehyde oxime derivatives. **2022**, 1265, 133339 0
- 281 Importance of R-CH<sub>3</sub>?O tetrel bonding and vinyl?aryl stacking interactions in stabilizing the crystal packing of 2,4-dihydroxy-3-methoxychalcone: Exploration of antileishmanial activity and molecular docking studies. **2022**, 1265, 133357 0
- 280 Four-Coordinate Monoboron Complexes with 8-Hydroxyquinolin-5-Sulfonate: Synthesis, Crystal Structures, Theoretical Studies, and Luminescence Properties. **2022**, 12, 783 1
- 279 Crystal structure elucidation, Hirshfeld surface analysis, lattice energy frame work, and molecular docking studies of copper(II) complex of 1-(3-bromo-5-chloro-2-hydroxyphenyl)ethan-1-one in the presence of solvent pyridine as secondary ligand. 1-13
- 278 Investigation on the growth, structural, vibrational, SHG behaviour and DFT studies of imidazolium hydrogen succinate single crystal. 0
- 277 DFT, lattice energy and Hirshfeld surface analysis of some 6-chloro-coumarin structures. 1-17
- 276 New Cu<sup>2+</sup> Complexes with N-Sulfonamide Ligands: Potential Antitumor, Antibacterial, and Antioxidant Agents. **2022**, 27, 3338 1
- 275 Theoretical Prediction of Structures and Properties of 2,4,6-Trinitro-1,3,5-Triazine (TNNTA) Green Energetic Materials from DFT and ReaxFF Molecular Modeling. **2022**, 15, 3873
- 274 Classical Intermolecular Hydrogen Bonding Motifs of Heterocyclic rac-2-Amino-3-carbonitrile Derivatives: Linking Hirshfeld Surface Analysis, CT-DNA Binding Affinity, and Molecular Docking. 0

273	Structural and computational analysis, spectroscopic and electrochemical elucidation of a Schiff base.	2
272	Novel hydrazone-2-iminothiazolidin-4-ones based on a monoterpene skeleton as potential antitumor agents: Synthesis, DFT studies, in vitro cytotoxicity, apoptosis inducing properties and molecular docking.	0
271	The effect of structural configuration on the DNA binding and in vitro antioxidant properties of new copper(II) N <sub>2</sub> O <sub>2</sub> Schiff base complexes.	0
270	Structure and surface analyses of a newly synthesized acyl thiourea derivative along with its in silico and in vitro investigations for RNR, DNA binding, urease inhibition and radical scavenging activities. <b>2022</b> , 12, 17194-17207	1
269	Zn(II) complexes with thiazolylhydrazones: structure, intermolecular interactions, photophysical properties, computational study and anticancer activity.	0
268	Combined Computational/Experimental Investigation of new cocrystals of the drug bosentan.	2
267	Engineering of a kinetically driven phase of phenoxazine by surface crystallisation.	2
266	Crystal structures of three zinc(II) halide coordination complexes with quinoline N-oxide. <b>2022</b> , 78,	
265	Noncovalent Interactions and Crystal Structure Prediction of Energetic Materials. <b>2022</b> , 27, 3755	
264	Syntheses and crystal structures of a nitroanthraceneboxazole and its oxidation product. <b>2022</b> , 78,	
263	Synthesis, Structural, Spectroscopic, and Hirshfeld Surface Analysis, and DFT Investigation of Benzaldehyde Semicarbazone. <b>2022</b> , 2022, 1-14	
262	Experimental Spectroscopic, Structural (Monomer and Dimer), Molecular Docking, Molecular Dynamics Simulation and Hirshfeld Surface Analysis of 2-Amino-6-Methylpyridine. 1-31	1
261	Synthesis, crystal structure analysis, DFT calculations, antioxidant and antimicrobial activity of N,N-di-2,4-dimethoxybenzyl-N'-2-nitrobenzoylthiourea. <b>2022</b> , 133579	1
260	Extensive Analyses on Expanding the Scope of Acid-Aminopyrimidine Synthons for the Design of Molecular Solids.	1
259	Topological and DFT studies of 8-hydroxyquinoline derivative and its copper complex having supramolecular interactions network. <b>2022</b> , 1214, 113791	
258	New insight into two penta-coordinated multinuclear copper(II) single-armed salamo-based complexes. <b>2022</b> , 540, 121047	2
257	Structure and optical properties of new nitro-derivatives of 2-N-alkylamino-picoline N-oxide isomers. <b>2022</b> , 1265, 133372	
256	Synthesis, crystal structure and ATR-FTIR, FT-Raman and UV-Vis spectroscopic analysis of dihydrochalcone (3R)-3-(4-chlorophenyl)-3-hydroxy-1-(2-hydroxyphenyl)propan-1-one. <b>2022</b> , 1266, 133516	1

- 255 Structural characterization and computational investigations of three fluorine-containing ligands with a terphenyl core. **2022**, 1266, 133474
- 254 Electrical, optical, and mechanical properties of modified Czochralski grown organic 4-nitrobenzaldehyde single crystal. **2022**, 169, 110839
- 253 Two Birds with One Stone: Simultaneous Harmless Ionization of Cfc and Resource Utilization of Waste Solar Panel Through One-Pot Hydrothermal Treatment.
- 252 Computational, Spectral and Structural Studies of New Hydrazinium Hydrogen Phthalate Monohydrate Salt. **2022**, 34, 2133-2140
- 251 Discovery and characterization of new crystal forms of bio-based nylon 4F salt.
- 250 Flexible organic crystals. Understanding the tractable co-existence of elastic and plastic bending. 5
- 249 Centroid-centroid and hydrogen bond interactions as robust supramolecular units for crystal engineering: X-ray crystallographic, computational and urease inhibitory investigations of 1,2,4-triazolo[3,4-a]phthalazines. 0
- 248 Supramolecular Dimeric Silver(I) Complex Based on the 1,1'-Bis(diphenylphosphino)ferrocene: Thermal Behaviors, Luminescence Studies and Cytotoxic Properties.
- 247 Hydrated magnesium (II) with H-bonded hexamethylenetetramine and co-ligands: synthesis, structural characterization, thermal decomposition, and hirshfeld surface analysis.
- 246 Synthesis, crystal structure, and antidiabetic property of hydrazine functionalized Schiff base: 1,2-Di(benzylidene)hydrazine. **2022**, 13, 234-240 1
- 245 Describing auxin solid state intermolecular interactions using contact descriptors, shape property and molecular fingerprint: comparison of pure auxin crystal and auxin-TIR1 co-crystal. **2022**, 13, 172-179
- 244 Antiparallel  $\pi$ - $\pi$  and C-H $\cdots$ O Contacts in a Novel Zn(II) Coordination Solid involving Hole Tetrel Bonding Interactions: A Combined Experimental and Theoretical Study, Hirshfeld Surface Analysis, Molecular Docking and Potential Drug Property.. **2022**, 133686 1
- 243 Synthesis, crystal structure and Hirshfeld surface analysis of a zinc(II) coordination polymer of 5-phenyl-1,3,4-oxadiazole-2-thiolate. **2022**, 78,
- 242 Anions Distorting Triggering Ferroelectricity in a Molecular Crystal □
- 241 Synthesis, crystal structure determination and Hirshfeld surface analysis of three new salt forms of creatinine with hydrobromic acid, 3-aminobenzoic acid and 3,5-dinitrobenzoic acid. **2022**, 78,
- 240 Crystal structure, Molecular structural analysis, Optical absorption and Thermal analysis of 2-amino-6-methyl pyridine-1-ium 2-carboxy-6-nitro benzoate [A third harmonic nonlinear optical organic single crystal. **2022**,
- 239 Synthesis, characterization, and thermal and computational investigations of the l-histidine bis(fluoride) crystal. **2022**, 28,
- 238 Vibrational spectroscopic signatures, effect of rehybridization and hyperconjugation on the dimer molecule of N-(4-chlorophenyl)-4,6-diaminopyrimidin-2(1H)-one-sulfanyl]acetamide- quantum computational approach. 1-17

- 237 Synthesis, X-Ray Crystallography and HF/DFT analysis of N(diethylcarbamothioyl) furan-2-carboxamide, Analyzed by Experimental and Theoretical Methods. **2022**, 133721
- 236 A silver(I) coordination polymer with bridging bis(thiosemicarbazone) ligands and unsupported argentophilic interactions. 1-11
- 235 Synthesis, Crystal Structure, Hirshfeld Surface Analysis, Molecular Docking, IR Spectroscopy and DFT Calculations of a Novel 2D Layered Hybrid Compound (C<sub>6</sub>H<sub>10</sub>N<sub>3</sub>O)<sub>2</sub>Cu<sub>2</sub>Cl<sub>6</sub>.
- 234 Phonon-Suppressing Intermolecular Adhesives: Catechol-Based Broadband Organic THz Generators. 2201391 3
- 233 Syntheses, Crystal structures, Theoretical studies, and Anticancer properties of an unsymmetrical Schiff base ligand N-2-(6-methylpyridyl)-2-hydroxy-1-naphthaldimine and its Ni(II) complex. **2022**, 133717 0
- 232 Synthetic approach to achieve halo imine units: Solid-state assembly, DFT based electronic and non linear optical behavior. **2022**, 803, 139843 6
- 231 The effect of halo-substituents on physical properties based on 1,3,5-triarylbenzenes: Synthesis, crystal structure and Hirshfeld surface. **2022**, 1267, 133606 0
- 230 Structure-Property Relationship of Three 2-Chloro-4-fluoro Chalcone Derivatives: A Comprehensive Study on Linear and Non-linear Optical Properties, Structural Characterizations and Density Functional Theory. **2022**, 1267, 133584 0
- 229 Synthesis, spectroscopic characterization, single crystal XRD, Hirshfeld Surface analysis and theoretical studies (DFT) of 4-adamantyl-(2-(substitutedbenzylidene)hydrazinyl)thiazoles. **2022**, 1267, 133620 4
- 228 Synthesis, single crystal X-ray, DFT, Hirshfeld surface and molecular docking studies of 9-(2,4-dichlorophenyl)-4a-hydroxy-tetramethyl-octahydro-1H-xanthene-1,8(2H)-dione. **2022**, 1268, 133613 3
- 227 Structural elucidation of phenoxybenzaldehyde derivatives from laboratory powder X-ray diffraction: A combined experimental and theoretical quantum mechanical study. **2022**, 1268, 133697 1
- 226 H<sub>2</sub>O brace molecules to slip stack: Transform ACQ to AIE for latent fingerprints recognition. **2022**, 450, 137933 0
- 225 New N-pyrimidinyl stilbazolium crystals for second-order nonlinear optics. **2022**, 156, 108454 1
- 224 Novel CuI coordination polymer self-assembled from 2,5-bis(pyridin-4-yl)-1,3,4-oxadiazole and thiocyanate ions: Synthesis, structural characterization, Hirshfeld surface analysis, thermal and magnetic studies. **2022**, 133790
- 223 Structural Features of the Cu(II) Complex with 5-Phenyltetrazolate Anion and 4,4'-Dimethyl-2,2'-bipyridine. **2022**, 67, 575-580
- 222 Decarbonylated bis-phosphine complexes bearing a Fe-Sn bond: NMR spectroscopy, X-Ray Structures, Hirshfeld Surface Analysis, and DFT Calculations. **2022**, 133754 1
- 221 X-ray structure analysis of the cholesterol 25- and 20-hydroperoxides, the elusive primary sidechain autoxidation products of cholesterol. **2022**, 187, 109092
- 220 Crystal structure, Hirshfeld surface analysis and DFT calculations of (E)-3-[1-(2-hydroxyphenyl)anilino]ethylidene]-6-methylpyran-2,4-dione. **2022**, 78, 864-870

- 219 Construction of a photoluminescent Zn(II)-based 2D MOF via in situ cis-trans isomerization of cis,cis-muconate ligand. **2022**, 134011
- 218 Unravelling the Structure of Peroxides with Antiparasitic Activity: The Relative Impact of a Trioxolane or a Tetraoxane Pharmacophore on the Overall Molecular Structure. **2022**, 87,
- 217 Crystal structure, Hirshfeld surface analysis and geometry optimization of 2-hydroxyimino-N-[1-(pyrazin-2-yl)ethylidene]propanohydrazide. **2022**, 78,
- 216 Crystal structure, Hirshfeld surface analysis and DFT calculations of 7-bromo-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one. **2022**, 78,
- 215 Synthesis, crystal structure and dft study of benzenesulfonamide compounds 1-ethyl-4-(phenylsulfonyl)piperazine and 1-((3-bromophenyl)sulfonyl)-4-methylpiperazine. 1-11
- 214 Structural and Molecular Packing study of Three New Amidophosphoric Acid Esters and Assessment of Their Inhibiting Activity Against SARS-CoV-2 by Molecular Docking. **2022**, 7,
- 213 One Pot Efficient Synthesis of 1,3-di(Naphthalen-1-yl)Thiourea; X-Ray Structure, Hirshfeld Surface Analysis, Density Functional Theory, Molecular Docking and In-Vitro Biological Assessment. **2022**, 133989 1
- 212 Exploring Highly Functionalized Tetrahydropyridine as a Dual Inhibitor of Monoamine Oxidase A and B: Synthesis, Structural Analysis, Single Crystal XRD, Supramolecular Assembly Exploration by Hirshfeld Surface Analysis, and Computational Studies. **2022**, 7, 29452-29464 1
- 211 X-ray structure, hirshfeld surfaces and interaction energy studies of 2,2-diphenyl-1-oxa-3-oxonia-2-boratanaphthalene. **2022**, 8, e10151 1
- 210 Synthesis, crystal structure, Hirshfeld surface analysis, energy frameworks and computational studies of Schiff base derivative. **2022**, 8, e10047 0
- 209 Quantitative Intermolecular Interactions Analysis and Magnetic Properties of Thiocyanatoiron(II) Complex with Nicotinamide Ligand. 0
- 208 Thermal and kinetic analysis of a new hydrazone-oxime ligand and its cadmium(II) complex: Synthesis, spectral characterization, crystallographic determination and Hirshfeld surface analysis. **2022**, 133887
- 207 Highly efficient hole transport derivatives based on fluoranthene core for application in perovskite solar cells. **2022**, 805, 139938
- 206 Synthesis, crystal structure and Hirshfeld surface analysis of 3-butyl-4-oxo-3,4-dihydroquinazoline-6-sulfonamide. **2022**, 41, 100926
- 205 New complexes of indium(III) diaryldithiophosphates: Structural characterization and insight into supramolecular interactions. **2022**, 226, 116094
- 204 2D polymeric lanthanide(III) compounds based on novel bright green emitting enaminone ligand. **2022**, 542, 121107 0
- 203 Experimental and computational analyses of the cocrystal of tetrahydrofuran-2,3,4,5-tetracarboxylic acid and urea. **2022**, 1269, 133820 0
- 202 Structural, vibrational characterization and DFT calculations of urea: DL-malic acid (1:1)  $\beta$ -crystal. **2022**, 1270, 133930 0

201	Synthesis, structure elucidation, Hirshfeld surface analysis, energy frameworks and DFT studies of novel ethyl 2-(5-methyl-2-oxopyridin-N-yl)acetate (OPA). <b>2022</b> , 1270, 133928	2
200	Synthesis, characterization, and x-ray crystallography of unexpected chloro-substitution on 1-(4-chlorophenyl)-3-phenylthiourea platinum(II) complex with tertiary phosphine ligand. <b>2022</b> , 1270, 133985	6
199	Structural, spectroscopic and quantum chemical analysis of an exocyclic extended double-bonded chalcone single crystal, with pharmaceutical scanning for breast cancer using MCF-7 cell line and EGFR domain target. <b>2022</b> , 1270, 133849	
198	A systematic study of the third-order nonlinear optical co-crystal of bis-((diisopropyl)ammonium) dichromate: X-ray, Hirshfeld surface, Optical, and Mechanical analysis. <b>2022</b> , 1270, 133869	0
197	Synthesis, spectroscopic characterization, biological activities, X-ray diffraction and molecular docking studies of 2-methyl-3-(thiazol-2-ylcarbamoyl)phenylacetate. <b>2022</b> , 1270, 133937	
196	Spectral, crystallographic, theoretical, and catalytic activity studies of the Pd(II) complexes in different coordination modes of benzoylthiourea ligand. <b>2022</b> , 1269, 133839	0
195	Exploring dithiolate-amine binary ligand systems for the supramolecular assemblies of Ni(II) coordination compounds: Crystal structures, theoretical studies, cytotoxicity studies, and molecular docking studies. <b>2022</b> , 543, 121157	0
194	A multidisciplinary study for investigating the interaction of an iron complex with bovine liver catalase.	0
193	Synthesis, crystal structure elucidation and interactions in 1,2,4,5-tetraazaspiro[5.5]undecane-3-thione: Hirshfeld surface analysis, 2d fingerprint plots and 3D energy framework calculations. <b>2022</b> , 41, 100933	0
192	Analysis of solid-liquid equilibrium behavior of highly water-soluble beet herbicide metamitron in thirteen pure solvents using experiments and molecular simulations. <b>2022</b> , 366, 120121	0
191	Investigation of solid-liquid equilibrium and thermodynamic models of D-Tagatose in mono-solvents and binary solvents. <b>2022</b> , 8, 100084	0
190	3D supramolecular assembly of Cu(II) CP containing 1D zig-zag chain and 2D paddle-wheel net: Structural elucidation and investigation of band gap. <b>2022</b> , 543, 121206	0
189	Synthesis, characterization, and biological properties of mono-, di- and poly-nuclear bismuth(III) halide complexes containing thiophene-2-carbaldehyde thiosemicarbazones. <b>2022</b> , 237, 111987	0
188	Simultaneous harmless ionization of CFC and resource utilization of waste solar panel through one-pot hydrothermal treatment. <b>2023</b> , 441, 129918	0
187	Molecular structure analysis of 4-fluoro phenyl(4-methyl piperidin-1-yl) methanone and a comparative study of its optical, antimicrobial and antioxidant activities with 4-chloro phenyl (4-methyl piperidin-1-yl) methanone. <b>2023</b> , 1271, 134080	0
186	Structural characterization (XRD, FTIR) and magnetic studies of Cd(II)-Sulfamethoxazole-2,2'-bipyridine: DFT and Hirshfeld Surface Analysis. <b>2023</b> , 1271, 133945	0
185	Studies on New Imidazo[2,1-b][1,3,4]thiadiazole Derivatives: Molecular Structure, Quantum Chemical Computational, and In silico Study of Inhibitory Activity Against Pim-1 Protein by using Molecular Modelling Methods and ADMET Profiling. <b>2023</b> , 1272, 134161	0
184	Structural insights, spectral, fluorescence, Z-scan, C-H...N-H hydrogen bonding and AIM, RDG, ELF, LOL, FUKUI analysis, NLO activity of N-2(Methoxy phenyl) acetamide. <b>2023</b> , 1272, 134140	1

- 183 Structural and spectroscopic characterization of the products formed in aqueous solution of hydrazine and maleic acid. **2023**, 1271, 134077 ○
- 182 The Crystal Structure, Hirshfeld Surface interactions, optical/Nonlinear Optical properties and evaluation of the antioxidant activity of 8-(3-chloropropanamido)quinolin-1-ium chloride: Experimental and theoretical studies. **2023**, 1271, 134014 ○
- 181 Unravelling the semiconductor properties of mixed stack donor acceptor cocrystals of pyrene derivatives and TCNQ: effect of crystal packing versus super-exchange mechanism. **2022**, 24, 6579-6586 ○
- 180 Recent advances in studying the nonnegligible role of noncovalent interactions in various types of energetic molecular crystals. **2022**, 24, 6119-6136 1
- 179 Unravelling supramolecular features and opto-electronic properties of a binary charge transfer cocrystal of a blue fluorescent di-carbazole and TFT. **2022**, 24, 6669-6676 ○
- 178 A comprehensive study on the photophysical and non-linear optical properties of thienyl-chalcone derivatives. **2022**, 24, 21927-21953 ○
- 177 Structural investigations and theoretical insights of a polymethoxy chalcone derivative: Synthesis, crystal structure, 3D energy frameworks and SARS CoV-2 docking studies. **2023**, 1272, 134226 ○
- 176 Crystal morphology prediction and experimental verification of venlafaxine hydrochloride. **2022**, 37, 133-142 ○
- 175 Crystal structure determination, Hirshfeld surface, crystal void, intermolecular interaction energy analyses, as well as DFT and energy framework calculations of 2-(4-oxo-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-1-yl)acetic acid. **2022**, 78, 953-960 ○
- 174 Spontaneous Isomerization [trans-B20H18]2 ↔ [iso-B20H18]2 during Cobalt(II) Complexation with Phenanthroline. **2022**, 67, 1169-1177 ○
- 173 New organic 4-(4-methoxystyryl)-1-methylpyridinium crystals for nonlinear optical applications. ○
- 172 Diastereomerically pure (S)- verbenone-isoxazoline hybrids: Synthesis, molecular structure, Hirshfeld surface analysis, density functional theory, cytotoxic effect, and apoptosis induction. ○
- 171 Synthesis, crystal structure, Hirshfeld surface, nonlinear optical properties and computational studies of Schiff based (E)-N'-(2,4-dimethoxybenzylidene) benzohydrazide single crystals for optoelectronic applications. **2022**, 54, ○
- 170 Differential study on the transition from a new polyhalogen-substituted unsymmetric salamo-based ligand to its Cu(II) and Co(II) complexes. 1-17 ○
- 169 Crystal polymorphism in 2,2'-bipyrimidine-based iridium(III) complexes. 1-13 ○
- 168 Copper 4-chlorobenzoate with isonicotinamide: synthesis, crystal structure, optical characterization and anticancer and cytotoxic properties. ○
- 167 Synthesis and Chemical Exploration of an Organic Exocyclic Chalcone Derivative for Its Therapeutic Proficiency against Breast Cancer. 1-19 ○
- 166 Solid-State and Aggregate Emission of Aroyl-S,N-Ketene Acetals are Controlled and Tuned by their Substitution Pattern. ○

- 165 Structure-elucidation of a bimetallic Hydroxo bridged Cu (II)-flufenamate-bpy complex and cytotoxic evaluation against MDAMB231 and A549 carcinoma cell lines. 0
- 164 Synthesis, crystal structure and Hirshfeld surface analysis of (1H-benzimidazol-2-yl)(morpholin-4-yl)methanethione. **2022**, 78, 999-1002 0
- 163 Xanthine oxidase inhibitory study of eight structurally diverse phenolic compounds. 9, 1
- 162 Structure and Spectroscopy of Iron Pentacarbonyl, Fe(CO)<sub>5</sub>. **2022**, 144, 17376-17386 0
- 161 Copper Complexes of 1,4-Naphthoquinone Containing Thiosemicarbazide and Triphenylphosphine Oxide Moieties; Synthesis and Identification by NMR, IR, Mass, UV Spectra, and DFT Calculations. **2022**, 7, 34463-34475 1
- 160 Penta-coordinated Cr(II) and Cu(II) complexes appended with 4'-(4-quinolyl)-2,2':6',2'-terpyridine: crystal structure, Hirshfeld Surface analysis, luminescence and thermal properties. **2022**, 134245 0
- 159 ANALYSIS OF THE CRYSTAL STRUCTURE AND ENERGY FRAMEWORKS OF 5-ACETIL-1,3-DIMETHYL BARBITURIC ACID. 0
- 158 Synthesis, crystal structures, and Hirshfeld analysis of three hexahydroquinoline derivatives. **2022**, 78, 0
- 157 Synthesis, X-ray and DFT Studies of 6-halo-3-(hydroxymethyl)cinnolin-4(1H)-ones. 1
- 156 Synthesis, X-Ray Diffraction, DFT and Hirshfeld Surface Studies of 9-(4-Hydroxyphenyl)-Tetramethyl-Hexahydro-1H-Xanthene-1,8(2H)-Dione. 1-24 0
- 155 DFT, Molecular Docking, Molecular Dynamics Simulation (MMGBSA) and Hirshfeld Surface Analysis of 5-Sulfosalicylic Acid. **2022**, 134242 0
- 154 Theoretical analysis of the effects of counterions on the supramolecular arrangement of sulfamethoxazole. **2022**, 28, 0
- 153 Improved solubility and hygroscopicity of enoxacin by pharmaceutical salts formation with hydroxybenzoic acids via charge assisted hydrogen bond. **2022**, 134272 0
- 152 Gefitinib-Resveratrol Cocrystal with Optimized Performance in Dissolution and Stability. **2022**, 1
- 151 Directional Self-Assembly of Ofloxacin and Syringic Acid: The First Salt Cocrystal of Ofloxacin with Phenolic Acid Displays Superior In Vitro/Vivo Biopharmaceutical Property and Enhanced Antibacterial Activity. 0
- 150 Synthesis, characterization, Hirshfeld surface analysis, and the study of antimicrobial, and acaricidal properties of copper(II) complexes with 2-(hydroxymethyl)benzimidazole ligand. **2022**, 227, 116146 0
- 149 One-pot synthesis, X-ray crystal structure, and identification of potential molecules against COVID-19 main protease through structure-guided modeling and simulation approach. **2022**, 15, 104230 1
- 148 Crystal engineering of a co-crystal of antipyrine and 2-chlorobenzoic acid: relative energetic contributions based on multipolar refinement. 0



- 147 Narrowing the band of green emission in manganese hybrids by reducing the hydrogen bond strength and structural distortion. 1
- 146 DNA binding, antitubercular, antibacterial and anticancer studies of newly designed piano-stool ruthenium(II) complexes. **2022**, 51, 16371-16382 1
- 145 Synthesis, crystal structure, exploration of the supramolecular assembly through Hirshfeld surface analysis and bactericidal activity of the cadmium organometallic complexes obtained from the heterocyclic ligand. **2022**, 4, 100600 4
- 144 Theoretical seeking of the charge transport materials with inherent mobility higher than 2,6-Diphenyl anthracene: three isomers of 2,6-Dipyridyl anthracene. 0
- 143 Synthesis, Structural Characterization and Hirshfeld Analysis of Ag(I), Au(I), Cd(II) and Hg(II) Complexes Containing Hemilabile- Ferrocenylbisphosphine [Fe{C<sub>5</sub>H<sub>4</sub>P(C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>NMe<sub>2</sub>-o)<sub>2</sub>]<sub>2</sub>. 0
- 142 A New Class of Organic Crystals with Extremely Large Hyperpolarizability: Efficient THz Wave Generation with Wide Flat-Spectral-Band. 2209915 0
- 141 Isomeric effect in structural studies of substituted nitro hydroxy-3-methoxy-benzaldehyde and nitro 2,3-dimethoxy-benzaldehyde derivatives.. **2022**, 134436 0
- 140 Crystal structure, growth, spectral, Hirshfeld surface, optical, thermal and third harmonic nonlinear optical studies of 2-amino-6-methyl pyridine-1-ium acetamido acetate monohydrate single crystal. 0
- 139 Anion-directed structural diversification in four new Cd(II) compounds of a flexible polyether-based dicarboxylic acid. **2022**, 110109 0
- 138 A detailed experimental and computational study of Cd complexes with pyridyl-based thiazolyl-hydrazones. 0
- 137 Synthesis and crystal structure of 2-(1,3-dithietan-2-ylidene)cyclohexane-1,3-dione. **2022**, 78, 1118-1121 0
- 136 Pyromellitate Ligand as Building Blocks in the Synthesis of Metal-Organic Frameworks with Hydroxyalkylamines. 0
- 135 Synthesis, crystal structure and Hirshfeld surface analysis of aqua(3-methoxycinnamato- $\mu$ )bis(1,10-phenanthroline- $\kappa^2$ N,N')cobalt(II) nitrate. **2022**, 78, 1113-1117 0
- 134 Bromine Substitution Effect on Structure, Reactivity, and Linear and Third-Order Nonlinear Optical Properties of 2,3-Dimethoxybenzaldehyde. **2022**, 126, 7852-7863 0
- 133 Exploring Polymorphism and Diversity in Intermolecular Interactions in Substituted Crystalline Benzophenones. **2022**, 22, 6686-6702 0
- 132 Structure-Directing Interplay between Tetrel and Halogen Bonding in Co-Crystal of Lead(II) Diethyldithiocarbamate with Tetraiodoethylene. **2022**, 23, 11870 0
- 131 Insights on sustainable fuels: a new benzimidazole derivative with potential as a diesel-biodiesel blend additive. 1-14 0
- 130 Design and Validation of Isomorphic Crystal Library for Nonlinear Optics and THz Wave Generation. 2201420 0

- 129 Synthesis, Structural, and Intriguing Electronic Properties of Symmetrical Bis-Aryl- $\beta,\beta$ -Unsaturated Ketone Derivatives. **2022**, 7, 39294-39309 5
- 128 Synthesis, characterization, DFT calculations and bromoperoxidase activity of binuclear oxidovanadium complexes containing vitamin B6. 1-22 0
- 127 Synthesis, Characterization and DFT Study of a New Family of High-Energy Compounds Based on s-Triazine, Carborane and Tetrazoles. **2022**, 27, 7484 0
- 126 Structural characterization, 3D-interaction energy and in-vitro antimicrobial studies of 1-(2-chloroacetyl)-3,5-dimethyl-2,6-bis(3,4,5-trimethoxyphenyl)piperidin-4-one. **2022**, 134462 0
- 125 2,6-disubstituted imidazothiadiazole 5-carbaldehyde: Synthesis, crystal structure elucidation and in-silico studies. **2022**, 42, 100962 0
- 124 2,4-Bis(2,4-dimethoxyphenyl)-1,3-dithia-2,4-diphosphetane 2,4-disulfide and its derivatives: Syntheses, structural characterizations, anticancer activities, and theoretical studies on some dithiophosphonato Ni(II) complex. **2023**, 1272, 134197 0
- 123 3,3'-[succinylbis(diazaneyl)]bis(N,N,N-trimethylpropan-1-ammonium) perchlorate: Synthesis, characterization, computational studies and in vitro anticancer activity against the human colon carcinoma cell line (HT-29). **2023**, 1273, 134377 0
- 122 Quantitative analysis of intermolecular interactions in crystalline substituted triazoles. **2023**, 1273, 134380 0
- 121 Synthesis and structural studies on the supramolecular architecture of two novel proton transfer molecular salts of 2 $\beta$ aminopyridine. **2023**, 1274, 134426 0
- 120 DFT guided substitution effect on azomethine reactive center in newly synthesized Schiff base aromatic scaffolds; syntheses, characterization, single crystal XRD, Hirshfeld surface and crystal void analyses. **2023**, 1273, 134215 0
- 119 Cation-controlled capture of polyoxovanadate-based organic/inorganic 1D architectures. 1
- 118 Experimental and computational studies on pseudotetrahedral nickel(II)-(R or S)-dihalogen-salicylaldiminates with R or R chirality induction at-metal. 0
- 117 Green synthesis, X-ray crystallography, DFT and Hirshfeld analysis of C-2 symmetric 1,3-bis(4-ethylphenyl)triaz-1-ene. **2023**, 1274, 134523 0
- 116 Planarity is one of the essential requirements for fluorescence in Red Fluorescent Protein chromophore analogs. **2023**, 1274, 134481 0
- 115 Synthesis, characterization, theoretical studies and antioxidant and cytotoxic evaluation of a series of Tetrahydrocurcumin (THC)-benzylated derivatives. **2023**, 1273, 134355 0
- 114 Synthesis, Characterization, Crystal Structure and Computational Study of Third-Order NLO Properties of Schiff bases. **2022**, 7, 1 1
- 113 Novel Organotin(IV) Complexes of 2-[4-Hydroxy-3-((2-hydroxyethylimino)methyl)phenylazo]benzoic Acid: Synthesis, Structure, Noncovalent Interactions and In Vitro Antibacterial Activity. **2022**, 12, 1582 0
- 112 Exploring Solid-State Supramolecular Architectures of Penta(carboxymethyl)diethylenetriamine: Experimental Observation and Theoretical Studies. **2022**, 7, 0

- 111 Synthesis, structure, hirshfeld surface analysis, non-covalent interaction, and in silico studies of 4-hydroxy-1-[(4-nitrophenyl)sulphonyl]pyrrolidine-2-carboxylic acid. ○
- 110 2-((3-(4-Methoxyphenyl)-4,5-dihydroisoxazol-5-yl)methyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide. **2022**, 2022, M1488 ○
- 109 N-Cycloamino substituent effects on the packing architecture of ortho-sulfanilamide molecular crystals and their in silico carbonic anhydrase II and IX inhibitory activities. **2022**, 78, ○
- 108 Synthesis, Characterization, and X-ray Crystallography, of the First Cyclohexadienyl Trifluoromethyl Metal Complex ( $\eta^5\text{-C}_6\text{H}_7$ )Fe(CO)2CF3. **2022**, 27, 7595 ○
- 107 Single crystal structure feature and quantum mechanical studies of a new binuclear Bi (III) complex and its activity against Helicobacter pylori. **2022**, 146, 110207 ○
- 106 Giant Electrocaloric Effect in a Molecular Ceramic. ○
- 105 New charge-transfer complexes of 1,2,5-chalcogenadiazoles with tetrathiafulvalenes. ○
- 104 Investigation of the role of hydrogen bonding in ionic liquid-like salts with both N- and S-soft donors. ○
- 103 Crystal structure of 2-(morpholino)ethylammonium picrate monohydrate. **2023**, 79, 8-13 ○
- 102 Structure property relationship of two pyrazole derivatives: Insights from crystal structure and computational studies. **2023**, 1276, 134771 ○
- 101 Optimization of electron distribution for enhancing the SHG output using electron withdrawing substituents: evidence from imidazole-picrate hybrid model. **2023**, 1276, 134726 ○
- 100 Impact of surface free energy on two-dimensional crystallization. ○
- 99 Chlorine counterion effect into the supramolecular arrangement of phenylephrine solid state. **2022**, 113992 ○
- 98 Synthesis, characterization of some substituted Quinolines derivatives : DFT, Computational, in Silico ADME, Molecular Docking and Biological Activities. **2022**, 100977 ○
- 97 Determination of Intermolecular Interactions of Nicotinamide Liganded Complexes of Co(II), Cu(II), Ni(II) and Zn(II) 4-Formilbenzoates by Hirshfeld Surface Analysis and Investigation of Interaction Energies.. ○
- 96 Dichlorinated Organic-Salt Terahertz Sources for THz Spectroscopy. 2202027 ○
- 95 A first principles study of nonlinear optical properties of a quinoline derivative. ○
- 94 Precise Molecular Design for Two Parent BN-Pentacyclic Isomers Through Stitching Engineering Toward Extremely Sensitive Explosive Detection. 2202433 ○

- 93 Ethylenediamine control of the supramolecular chemistry of magnesium phthalocyanine. **2022**, 121362 ○
- 92 Simultaneous presence of mono- and bi-cationic bipyridyls within a metal-organic supramolecular host: crystal structure, spectral and Hirshfeld surface analysis. 1-13 ○
- 91 Synthesis, Structural Characterization, Hirshfeld Analysis and AIM Analysis of 2,4,8,10-tetra-tert-butyl-6-phenyldibenzo[d,g][1,3,6,2]-dioxaselenaphosphocine and its Oxide and Selenide Derivatives. ○
- 90 Synthesis of New Cobalt(III) Meso-Porphyrin Complex, Photochemical, X-ray Diffraction, and Electrical Properties for Photovoltaic Cells. **2022**, 27, 8866 ○
- 89 Heteroaryl-Substituted bis-Anils: Aggregation-Induced Emission (AIE) Derivatives with Tunable ESIPT Emission Color and pH Sensitivity. ○
- 88 Structurally Unique Salts of Cyamemazine and Their Pharmaceutical Implications. ○
- 87 Anticancer Agents as Design Archetypes: Insights into the Structure-Property Relationships of Ionic Liquids with a Triarylmethyl Moiety. ○
- 86 Investigations of stable penta- and hexa-coordinate polynuclear Zn(II) and Cd(II) complexes derived from a single-armed salamo-based ligand. 1-17 ○
- 85 Unraveling the Nature of Hydrogen Bonds of Proton Sponges Based on Car-Parrinello and Metadynamics Approaches. **2023**, 24, 1542 ○
- 84 Syntheses, crystal structure, luminescent properties and Hirshfeld surface of a set of triazole-based salts. **2023**, 134980 ○
- 83 Synthesis, Crystal Structure, DFT Studies on Tetramethyl-(p-Tolyl)-Hexahydro-1H-Xanthene-1,8(2H)-Dione. 1-23 ○
- 82 Pyridine derivatives complexes of Co (II) and Ni (II) 3-Bromobenzoates: Crystal Structure, in silico Anti-SARS-CoV-2 potential, Serum Albumin Binding Properties and Cytotoxicity. ○
- 81 Templating influence of regulated inorganic framework in two-dimensional ferroelastic perovskites: (C<sub>3</sub>H<sub>5</sub>CH<sub>2</sub>NH<sub>3</sub>)<sub>2</sub>[MCl<sub>4</sub>] (M = Mn and Cd). ○
- 80 Features of the Crystal Structure of Benzyl Derivatives of Triacanthine. Effect of Weak Interactions on the Formation of Stable Channel Type Solvates. ○
- 79 Efficient organic terahertz generator with extremely broad terahertz molecular vibrational mode-free range. **2023**, 11, 011101 ○
- 78 Synthesis, crystal structure and dielectric properties of a hybrid dihydrogen arsenate salt: (C<sub>9</sub>H<sub>11</sub>N<sub>4</sub>)H<sub>2</sub>AsO<sub>4</sub>. ○
- 77 Synthesis, structural analysis, DFT study, antioxidant activity of metal complexes of N-substituted thiourea. **2023**, 231, 116274 ○
- 76 Does one hydrogen atom matter? Crystal structures and spectroscopic studies of five-coordinate manganese porphyrin complexes. **2023**, 211, 111068 ○

- 75 Synthesis, crystal structure, electronic structure, and anti-tubercular properties of two new coumarin derivatives bearing theophylline moiety. **2023**, 1277, 134888 ○
- 74 Synthesis, crystal studies, antimicrobial activity, and BSA binding studies of metal complexes derived from pyridyl-based hydrazone: Multi-spectroscopic and DFT approach. **2023**, 175, 111191 ○
- 73 Comprehensive study of substituent effects on structure and photochromic properties of 1,3-benzoxazine-4-one spiropyrans. **2023**, 1277, 134898 ○
- 72 Crystal structure, host-guest interactions, and supramolecular features of a novel  $\pi$ -hydroxy bridged eclipsed dimer based on indium(III) tetrapyrazinoporphyrazine. ○
- 71 Insights into structure-property relationships in ionic liquids using cyclic perfluoroalkylsulfonylimides. ○
- 70 Anticooperativity and Competition in Some Cocrystals Featuring Iodine-Nitrogen Halogen Bonds. ○
- 69 Synthesis and crystal structure, Hirshfeld surface analysis, and DFT calculation of 2-((4-(1-benzyl-2-methyl-4-nitro-1H-imidazol-5-yl)piperazin-1-yl)methyl)-5-phenyl-1,3,4-oxadiazole. **2023**, 1280, 135069 ○
- 68 Structural and quantitative analysis of intermolecular solid-state interactions in cocrystals obtained from nucleobases and methylxanthines with gallic acid. **2023**, 1280, 135074 ○
- 67 Structural elucidation of 1:4:4 stoichiometric form of thymine-gallic acid cocrystal hydrate: Hirshfeld surface analysis, 3D energy framework, DFT calculations, and SARS CoV-2 docking studies. **2023**, 1280, 135072 ○
- 66 New supramolecular architectures of 4'-(4-quinolinyl)-2,2':6',2'-terpyridine based on tin complexes: Design, structural variations and thermal properties. **2023**, 1279, 135038 ○
- 65 Construction of 3D interpenetrated dual linker coordination polymers of Zn(II) by varying the length and flexibility of bis(pyridyl) linkers. **2023**, 1280, 135042 ○
- 64 Experimental and theoretical studies of a thiourea derivative: 1-(4-chloro-benzoyl)-3-(2-trifluoromethyl-phenyl)thiourea. **2023**, 1279, 134996 ○
- 63 A quinoline-benzotriazole derivative: Synthesis, crystal structure and characterization by using spectroscopic, DFT and molecular docking methods. **2023**, 5, 100916 ○
- 62 Effect of Changing Anion on the Crystalline Structure, Crystal Structure, Hirshfeld Surface, IR and NMR Spectroscopy of Organic Salts and Hybrid Compounds:  $C_6H_5NH_2$  and  $C_6H_5N_3$  ○
- 61 Crystal structures of (12E)-12-(4-benzylidene)-7,7,16-trimethyl-3-(4-methylphenyl)-1-oxa-16-azatetracyclo[11.2.1.0.2,11.0.4,9]hexadeca-2(11),4(12),12,13-tetraene and (12E)-12-(4-bromobenzylidene)-7,7,16-trimethyl-10-oxa-16-azatetracyclo[11.2.1.0.2,11.0.4,9]hexadeca-2(11),4(12),12,13-tetraene. **2023**, 1279, 135038 ○
- 60 Syntheses, crystal structures and Hirshfeld surface analyses of N-arylsulfonyl derivatives of cytosine. **2023**, 79, 313-318 ○
- 59 Experimental and theoretical analyses and investigation of intermolecular interactions and antibacterial activity of a novel proton transfer compound: 8-hydroxyquinolinium oxalate monohydrate. **2023**, 9, e14703 ○
- 58 Analysis of the dissolution behavior and solubility of Rotigotine form II in different mono-solvents. **2023**, 377, 121532 ○

- 57 Synthesis, single crystal structure determinations, Hirshfeld surface analysis, crystal voids, interaction energies, and density functional theory studies of functionalized 1,3-thiazoles. **2023**, 1281, 135108 ○
- 56 Zn(II) complexes with pyridyl-based 1,3-selen/thiazolyl-hydrazones: A comparative study. **2023**, 1281, 135193 ○
- 55 Cooperativity effects in a new pterostilbene/phenanthroline cocrystal. **2023**, 1282, 135227 ○
- 54 Structural, physicochemical and anticancer study of Zn complexes with pyridyl-based thiazolyl-hydrazones. **2023**, 1281, 135157 ○
- 53 Design and synthesis of piano-stool ruthenium(II) complexes and their studies on the inhibition of amyloid  $\beta$  (1-42) peptide aggregation. **2023**, 239, 124197 ○
- 52 Effect of the substituted location on luminescent behaviors with Ambroxol moieties: Synthesis, crystal structure and Hirshfeld surface. **2023**, 1284, 135328 ○
- 51 New semiconductor halocadmiate  $[CdnXm](2n\bar{n})$  crystal structure, molecular conformation and theoretical investigations. **2023**, 322, 123954 ○
- 50 Design, synthesis and characterization of a novel oxygen-containing heterocycle crystal with NLO properties. **2023**, 282, 170851 ○
- 49 A novel use of an oxime molecule as supramolecular tecton. Synthesis of a Pt (II) 2D network. **2023**, 1285, 135485 ○
- 48 On the structures of free-base lepidine and some mineral acid salts. **2023**, 1285, 135460 ○
- 47 Molecular modeling and solubility of olopatadine hydrochloride polymorphs. **2023**, 1224, 114110 ○
- 46 Synthesis, crystal structure, DFT calculations, and Hirshfeld surface analysis of an NNN pincer type compound. **2023**, 1283, 135252 ○
- 45 Praziquanamine enantiomers: Crystal structure, Hirshfeld surface analysis, and quantum chemical studies. **2023**, 1283, 135343 ○
- 44 Studies towards investigation of Naphthoquinone-based scaffold with crystal structure as lead for SARS-CoV-19 management. **2023**, 1283, 135256 ○
- 43 Arsenic-Involving Intermolecular Interactions in Crystal Structures: The Dualistic Behavior of As(III) as Electron-Pair Donor and Acceptor. **2023**, 23, 1033-1048 ○
- 42 Photocatalytic degradation of remdesivir nucleotide pro-drug using  $[Cu(1\text{-methylimidazole})_4(SCN)_2]$  nanocomplex synthesized by sonochemical process: Theoretical, hirshfeld surface analysis, degradation kinetic, and thermodynamic studies. **2023**, 222, 115321 1
- 41 Solvent Coligand-Induced Spin State Variation in Iron(II) Complexes Bearing Pentadentate N5 Ligand Toward the Construction of an N5O Spin Crossover Center. **2023**, 23, 1622-1632 ○
- 40 Effect of the Solvent on the Crystallographic and Magnetic Properties of Rhenium(IV) Complexes Based on 2,2'-Bipyrimidine Ligand. **2023**, 11, 78 ○

- 39 A 3D Coordination Polymer Based on Syn-Anti Bridged  $[Mn(RCOO)_2]_n$  Chains Showing Spin-Canting with High Coercivity and an Ordering Temperature of 14 K. **2023**, 9, 55 ○
- 38 Improving enzymatic performance of antioxidant enzyme catalase in combination with  $[Mn(phen)_2Cl_2O]Cl \cdot tu$  complex. **2023**, 37, ○
- 37 Effect of crystal packing on charge transfer in the heteroleptic gallium(III) complex. **2023**, 72, 193-201 ○
- 36 Single Crystal Investigations, Hirshfeld Surface Analysis, DFT Studies, Molecular Docking, Physico-Chemical Characterization, and Biological Activity of a Novel Non-Centrosymmetric Compound with a Copper Transition Metal Precursor. **2023**, 8, 7738-7748 ○
- 35 Halogen Bond-Involving Supramolecular Assembly Utilizing Carbon as a Nucleophilic Partner of  $I \cdots C$  Non-covalent Interaction. **2023**, 18, ○
- 34 Synthesis, Characterization, Crystal Structures, and Supramolecular Assembly of Copper Complexes Derived from Nitroterephthalic Acid along with Hirshfeld Surface Analysis and Quantum Chemical Studies. **2023**, 8, 8530-8540 ○
- 33 Magnetization Slow Dynamics in Mononuclear Co(II) Field-Induced Single-Molecule Magnet. **2023**, 23, 2430-2441 ○
- 32 Stability and Mechanical Properties of Darunavir Isostructural Solvates: An Experimental and Computational Study. **2023**, 23, 2905-2915 ○
- 31 Luminescence Enhancement and Temperature Sensing Properties of Hybrid Bismuth Halides Achieved via Tuning Organic Cations. **2023**, 28, 2380 ○
- 30 Synthesis, crystal structures, and DFT calculations: novel Mn(II), Co(II) and Ni(II) complexes of N-(pyridin-2-ylmethylene)methanamine with isothiocyanate as promising optical materials. **2023**, 55, ○
- 29 SYNTHESIS, CRYSTAL STRUCTURE, SUPRAMOLECULAR ASSEMBLY EXPLORATION BY HIRSHFELD SURFACE ANALYSIS AND COMPUTATIONAL STUDY OF 6-BROMO-2-OXO-2H-CHROMENE-3-CARBONITRILE (BOCC). **2023**, 64, 302-313 ○
- 28 Synthesis, Structure, Hirshfeld Surface Analysis, Non-Covalent Interaction, and In Silico Studies of 4-Hydroxy-1-[(4-Nitrophenyl)Sulfonyl]Pyrrolidine-2-Carboxylic Acid. ○
- 27 Near-IR Absorbers Based on Pt(II)-Dithiolene Donor-Acceptor Charge-Transfer (CT) Systems: A Structural Analysis to Highlight DA Interactions. **2023**, 28, 2566 ○
- 26 Solvatochromism and Reversible Solvent Exchange Phenomena in Solvatomorphic Organic Chromophore Crystals. **2023**, 23, 2922-2931 ○
- 25 Crystal structure of trimethyl({tris[(phenylsulfanyl)methyl]silyl}methoxy)silane and Hirshfeld surface analysis of 3-bromo-2,2-bis(bromomethyl)propan-1-ol. **2023**, 79, 323-327 ○
- 24 Sulfonamide derived Schiff base Mn (II), Co (II), and Ni (II) complexes: Crystal structures, density functional theory and Hirshfeld surface analysis. ○
- 23 Crystal structure and Hirshfeld surface analysis of mono/bis(aqua- $\mu$ )[N-(2-oxidobenzylidene)valinato- $\beta$  O,N,O?] $\mu$ copper(II): dimeric Schiff base copper(II) complexes having different numbers of coordinated water molecules. **2023**, 79, 361-366 ○
- 22 Novel pharmaceutical co-crystals of gefitinib: synthesis, dissolution, cytotoxicity, and theoretical studies. ○

- 21 Supramolecular Structure of Tris(1,10-phenanthroline)zinc(II)-Cation and N,N',N'-tris(carboxymethyl)-1,3,5-benzenetricarboxamide-Anion: Synthesis, Crystal Structure, Vibrational Spectra, and Theoretical Investigations. **2023**, 13, 569 ○
- 20 Synthesis, X-ray structure, DFT investigation, and molecular docking of 1,3,5-tricyclohexyl-1,3,5-triazinane-2,4,6-trione, a cyclic polyamide with anti HIV-1 (RT), antiplatelet, and anticoagulant activities. ○
- 19 New Insights into the Solubilization of Multicomponent Crystals: A Case Study of Pipemidic Acid. ○
- 18 Arylsulfonamide chalcones as alternatives for fuel additives: antioxidant activity and machine learning protocol studies. ○
- 17 Single-Crystal X-ray Diffraction Analysis of Inclusion Complexes of Triflate-Functionalized Pillar[5]arenes with 1,4-Dibromobutane and n-Hexane Guests. **2023**, 13, 593 ○
- 16 Phosphorus-Nitrogen compounds: part 70. Syntheses of tetraaminomono/bis(4-fluorobenzyl)spiro(N/N)cyclotriphosphazenes: structural characterization, Hirshfeld surface analysis and comparative evaluation of esterase activities of hCA I and hCA II bioenzymes. ○
- 15 Synthesis, Crystal Structure, Supramolecular Assembly Inspection by Hirshfeld Surface Analysis and Computational Exploration of 4-Phenyl-6-(p-Tolyl)Pyrimidin-2 (1H)-One (PPTP). **2023**, 64, 437-449 ○
- 14 2,4,8,10-Tetra-tert-butyl-6-phenyldibenzo[d,g]-[1,3,6,2]dioxaselenaphosphocine Complexes: C-Be Bond Cleavage and Its Oxidative Addition to Form a Novel Octahedral Rhodium(III) Complex and Hirshfeld Analysis. ○
- 13 An investigation into the Brønsted acidity of the perfluorinated alkoxy silanes {(F3C)3CO}3SiH and {(F6C5)3CO}2Si(Cl)H. ○
- 12 Hetero-Aggregation-Induced Tunable Emission in Multicomponent Crystals. ○
- 11 Novel Mononuclear Tetrabromonitrosylrhenate(II) Complexes Containing Azole-Type Ligands: Magnetostructural Characterization through Hirshfeld Surfaces Analysis. **2023**, 13, 658 ○
- 10 Synthesis, Crystal structure, Hirshfeld surface interactions, anti-corrosion analysis, DFT calculations, Docking studies and evaluation of the antioxidant activity of a new zwitterion Schiff base. **2023**, 1286, 135569 ○
- 9 Preparation and Characterization of N-benzyl-2-methyl-4-nitroaniline (BNA) Single Crystals by Physical Vapour Transport (PVT) Technique. **2023**, 135593 ○
- 8 SYNTHESIS, OPTICAL AND THERMAL ANALYSIS OF p-BROMO CHALCONE DERIVATIVES: A THEORETICAL AND EXPERIMENTAL STUDIES. **2023**, 135591 ○
- 7 Synthesis, X-ray, DFT, Hirshfeld surface analysis, molecular docking, urease inhibition, antioxidant, cytotoxicity, DNA protection, and DNA binding properties of 5-(tert-butyl)-N-(2,4-dichlorophenyl)-1H-1,2,4-triazol-3-amine. ○
- 6 Synthesis, crystal structure, Hirshfeld surface, biological evaluation, DFT and molecular docking studies of unsymmetrical 3-allyl-5-ethyl-1,4-dihydro-2,6-dimethyl-4-phenyl pyridine-3,5-dicarboxylate derivatives. ○
- 5 Synthesis, virtual screening, and computational approach of 6-(4-methoxyphenyl)-4-phenyl-1,2-dihydropyrimidin-2-one as a potential target for thioredoxin glutathione reductase (TGR). **2023**, 135623 ○
- 4 Crystal Structures of 3,3',5,5'-Tetrabromo-4,4'-bipyridine and Co(II) Coordination Polymer Based Thereon. **2023**, 13, 704 ○



- 3 Complex interplay of hydrogen bonding, halogen bonding and  $\pi$ -interactions in methyl 2-(7-chloro-1H-pyrazolo[3,4-b]quinolin-1-yl)acetate: Synthesis, X-ray crystallography, energetic features and anti-urease efficacy. **2023**, 135625 ○
- 2 Computational studies on optoelectronic and nonlinear optical properties of para-substituted nitrobenzofurazan compound. **2023**, 35, 106133 ○
- 1 Synthesis, X-ray diffraction and theoretical studies to understand the molecular basis of druglikeness of isoxazole analogs. **2023**, 1287, 135734 ○