

# The Cambridge Structural Database

Acta Crystallographica Section B: Structural Science, Crystal E  
72, 171-179

DOI: [10.1107/s2052520616003954](https://doi.org/10.1107/s2052520616003954)

Citation Report

#	ARTICLE	IF	CITATIONS
1	Solvent inclusion in the crystal structure of bis[(adamantan-1-yl)methanaminium chloride] 1,4-dioxane hemisolvate monohydrate explained using the computed crystal energy landscape. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1348-1352.	0.2	5
2	Crystal structures of three carbazole derivatives: 12-ethyl-7-phenylsulfonyl-7H-benzofuro[2,3-b]carbazole, (1), 2-(4,5-dimethoxy-2-nitrophenyl)-4-hydroxy-9-phenylsulfonyl-9H-carbazole-3-carbaldehyde, (2), and 12-phenyl-7-phenylsulfonyl-7H-benzofuro[2,3-b]carbazole, (3). Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1744-1750.	0.2	0
3	Crystal structure of (1S,3R,8R,10S)-2,2-dichloro-10-hydroxy-3,7,7,10-tetramethyltricyclo[6.4.0.01,3]dodecan-9-one. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 709-711.	0.2	0
4	Crystal structure of diaquabis(2-chloropyridine- $\hat{\nu}$ N)bis(thiocyanato- $\hat{\nu}$ N)nickel(II). Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1492-1494.	0.2	1
5	Crystal structure of 6,7-dihydroxy-6,7-dihydro-3H-imidazo[1,2-a]purin-9(5H)-one. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1147-1149.	0.2	0
6	Crystal structure of 5-[(4-carboxybenzyl)oxy]isophthalic acid. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1219-1222.	0.2	0
7	Crystal structure of a compact three-dimensional metal-organic framework based on Cs <sup>+</sup> and (4,5-dicyano-1,2-phenylene)bis(phosphonic acid). Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1794-1798.	0.2	1
8	Crystal structure of poly[bis(ammonium) [bis(1/4-benzene-1,3,5-tricarboxylato)dizincate] 1-methylpyrrolidin-2-one disolvate]. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 764-767.	0.2	1
9	Anisotropic compressibility of the coordination polymer emim[Mn(btc)]. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 389-394.	0.5	8
10	A synchrotron study of [5,10,15,20-tetrakis(3-cyanophenyl)porphyrinato- $\hat{\nu}$ 4N5,N10,N15,N20]copper(II) nitrobenzene trisolvate at 80 K. Acta Crystallographica Section C, Structural Chemistry, 2016, 72, 861-866.	0.2	0
11	A non-solvated form of [(Z)-O-methyl-N-(2-methylphenyl)thiocarbamato- $\hat{\nu}$ S](triphenylphosphane- $\hat{\nu}$ P)gold(I): crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1446-1452.	0.2	3
12	The Effect of Ligand Design on Metal Ion Spin State—Lessons from Spin Crossover Complexes. Crystals, 2016, 6, 58.	1.0	103
13	Synthesis and Crystallographic Characterization of a Maleimide Derivative of Tryptamine. Crystals, 2016, 6, 153.	1.0	6
14	Molecular structures of tris(1-tert-butyl-2-mercaptoimidazolyl)hydroborate complexes of titanium, zirconium and hafnium. Acta Crystallographica Section C, Structural Chemistry, 2016, 72, 806-812.	0.2	3
15	Crystal structure of 9,9- $\hat{\nu}$ 2-[(1E,1 $\hat{\nu}$ 2E)-[1,4-phenylenebis(azanylylidene)]bis(methanylylidene)]bis(2,3,6,7-tetrahydro-1H,5H-pyrido[3,2-b]quinolin-8-ol). Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1366-1369.	0.2	11
16	Disodium hydrogen citrate sesquihydrate, Na <sub>2</sub> HC <sub>6</sub> H <sub>5</sub> O <sub>7</sub> (H <sub>2</sub> O) <sub>1.5</sub> . Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 943-946.	0.2	11
17	Synthesis and X-ray Crystallography of [Mg(H <sub>2</sub> O) <sub>6</sub> ][AnO <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> COO) <sub>3</sub> ] <sub>2</sub> (An = U, Np, or Pu). Inorganic Chemistry, 2016, 55, 7688-7693.	1.9	20
18	Protein-Ligand Informatics Force Field (PLIFF): Toward a Fully Knowledge Driven Force Field for Biomolecular Interactions. Journal of Medicinal Chemistry, 2016, 59, 6891-6902.	2.9	24



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37	Mono urotropine adducts of some binary zinc xanthatates and dithiocarbamates: solid-state molecular structures and supramolecular self-assembly. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2016, 231, 737-747.	0.4	1
38	A second polymorph of sodium dihydrogen citrate, NaH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> : structure solution from powder diffraction data and DFT comparison. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 854-857.	0.2	17
39	Crystal structure of (1S,3R,8R,9R)-2,2-dichloro-3,7,7-trimethyl-10-methylenetricyclo[6.4.0.01,3]dodecan-9-ol. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 1163-1166.	0.2	0
40	Accurate dissociation energies of two isomers of the 1-naphthol...cyclopropane complex. <i>Journal of Chemical Physics</i> , 2016, 145, 164304.	1.2	19
41	Crystal structure of norgestimate, C <sub>23</sub> H <sub>31</sub> NO <sub>3</sub> . <i>Powder Diffraction</i> , 2016, 31, 274-278.	0.4	1
42	Synthesis, Electronic, Magnetic and Structural Characterization of New Trinuclear Mixed-Valence Co <sup>III</sup> Co <sup>II</sup> Co <sup>III</sup> Complex.. <i>ChemistrySelect</i> , 2016, 1, 6866-6871.	0.7	12
43	Structure of ionic liquids with cationic silicon-substitutions. <i>Journal of Chemical Physics</i> , 2016, 145, .	1.2	21
44	Crystal structure and fluorescence properties of catena-poly[[[2,2-bis(1H-imidazole- $\eta^2$ N,N $\eta^2$ )cadmium]-di- $\frac{1}{4}$ -chlorido]. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 1421-1424.	0.2	0
45	Monoclinic-to-orthorhombic phase transition of the hexamethylenetetramine-2-methylbenzoic acid (1/2) cocrystal with temperature-dependent dynamic molecular disorder. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2016, 72, 971-980.	0.2	3
46	Crystal structure of 3,5-dimethylpyridine-N-oxide dihydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 1687-1690.	0.2	1
47	Structural and theoretical characterization of a new twisted 4 $\eta^2$ -substituted terpyridine compound: 4 $\eta^2$ -(isoquinolin-4-yl)-2,2 $\eta^2$ :6 $\eta^2$ ,2 $\eta^2$ -terpyridine. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2016, 72, 932-938.		2
48	Crystal structure of tetrakis(isonicotinamide- $\eta^1$ N)bis(thiocyanato- $\eta^1$ N)cobalt(II) "isonicotinamide" ethanol (1/2/1). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 1077-1080.	0.2	5
49	Crystal structure of hexakis(dimethyl sulfoxide- $\eta^1$ O) manganese(II) diiodide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 904-906.	0.2	4
50	Reversible Dihydrogen Activation by Reduced Aryl Boranes as Main-Group Ambiphiles. <i>Angewandte Chemie</i> , 2016, 128, 14273-14277.	1.6	40
51	Different N $\cdots$ H... $\pi$ interactions in two indole derivatives. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 699-703.	0.2	4
52	Crystal structure of dichlorido{2-methyl-2-[(pyridin-2-ylmethyl)amino]propan-1-ol- $\eta^3$ N,N $\eta^2$ ,O}copper(II) from synchrotron data. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 1400-1403.	0.2	1
53	Ring-strain release in neutral and dicationic 7,8,17,18-tetrabromo-5,10,15,20-tetraphenylporphyrin: crystal structures of C <sub>44</sub> H <sub>26</sub> Br <sub>4</sub> N <sub>4</sub> and C <sub>44</sub> H <sub>28</sub> Br <sub>4</sub> N <sub>4</sub> <sup>2+</sup> ·2ClO <sub>4</sub> <sup>-</sup> ·3CH <sub>2</sub> Cl <sub>2</sub> . <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 824-828.	0.2	1
54	Bis[bis( <i>N</i> -2-hydroxyethyl, <i>N</i> -isopropyl-dithiocarbamato)mercury(II)] <sub>2</sub> : crystal structure and Hirshfeld surface analysis. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2016, 231, 403-413.	0.4	23

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55	Constructing chiral MOFs by functionalizing 4,2,6,4-terpyridine with long-chain alkoxy domains: rare examples of <i>neb</i> nets. <i>CrystEngComm</i> , 2016, 18, 4704-4707.	1.3	16
56	Hydrogen bonding at C=Se acceptors in selenoureas, selenoamides and selones. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 317-325.	0.5	23
57	Engineering and manufacturing of pharmaceutical co-crystals: a review of solvent-free manufacturing technologies. <i>Chemical Communications</i> , 2016, 52, 8772-8786.	2.2	111
58	New multi-component solid forms of anti-cancer drug Erlotinib: role of auxiliary interactions in determining a preferred conformation. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 291-300.	0.5	21
59	Structural, Hirshfeld surface and theoretical analysis of two conformational polymorphs of <i>N,N</i> -bis(pyridin-3-ylmethyl)oxalamide. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2016, 231, 415-425.	0.4	10
60	Supramolecular hydrogen-bonding patterns of co-crystals containing the active pharmaceutical ingredient (API) phloroglucinol and <i>N</i> -heterocycles. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 326-334.	0.5	7
61	The effect of thermal expansion on photoisomerisation in the crystals of $[\text{Co}(\text{NH}_3)_3]_5\text{NO}_2\text{Cl}(\text{NO}_3)_3$ : different strain origins <i>â€</i> different outcomes. <i>CrystEngComm</i> , 2016, 18, 7276-7283.	1.3	14
62	The development and use of a crystallographic database. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 167-168.	0.5	12
63	Cyanoacrylic- and (1-cyanovinyl)phosphonic acid anchoring ligands for application in copper-based dye-sensitized solar cells. <i>RSC Advances</i> , 2016, 6, 86220-86231.	1.7	11
64	Weak interactions in the crystal structures of two indole derivatives. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 964-968.	0.2	0
65	Crystal structures of 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(3-nitrophenyl)acetamide monohydrate and N-(2-chlorophenyl)-2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]acetamide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 1171-1175.	0.2	3
66	Accelerated structure-based design of chemically diverse allosteric modulators of a muscarinic G protein-coupled receptor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E5675-84.	3.3	82
67	Hydrogen bonding in the crystal structure of the molecular salt of pyrazole <i>â€</i> pyrazolium picrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 861-863.	0.2	7
68	The electronic and solvatochromic properties of $[\text{Co}(\text{L}(\text{bipyridine})_2)]^+ (\text{L} = \text{Tj ETQq1 1 0.784314 rgBT / Over Dalton Transactions}$ , 2016, 45, 15575-15585.	1.6	11
69	Anharmonic and Quantum Fluctuations in Molecular Crystals: A First-Principles Study of the Stability of Paracetamol. <i>Physical Review Letters</i> , 2016, 117, 115702.	2.9	59
70	One barbiturate and two solvated thiobarbiturates containing the triply hydrogen-bonded <i>ADA</i> synthon, plus one ansovate and three solvates of their cofomer 2,4-diaminopyrimidine. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2016, 72, 705-715.	0.2	4
71	Using crystal structure prediction to rationalize the hydration propensities of substituted adamantane hydrochloride salts. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 551-561.	0.5	15
72	The new coordination modes of bis(1,2,4-diazaphospholyl)methane. <i>Polyhedron</i> , 2016, 119, 325-334.	1.0	5

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73	Solid-state study of the structure and host-guest chemistry of cucurbituril-ferrocene inclusion complexes. <i>Dalton Transactions</i> , 2016, 45, 17042-17052.	1.6	12
74	Crystal structure and magnetic properties of unusual 3D cyanide bridged {[Cu(bapa)] <sub>3</sub> [Cr(CN) <sub>6</sub> ] <sub>2</sub> }·6nH <sub>2</sub> O (bapa= bis(3-aminopropyl)amine) network. <i>Polyhedron</i> , 2016, 119, 548-554.	1.0	3
75	One dimensional Mn(III) Schiff-base complex organization through very strong symmetrical H-bond interaction. <i>Inorganica Chimica Acta</i> , 2016, 453, 692-696.	1.2	4
76	Dehydration of $\beta$ -oxalic acid dihydrate: Structural, spectroscopic and thermal study with implications on the disruption of water molecular bridges in soil organic matter. <i>Thermochimica Acta</i> , 2016, 643, 73-82.	1.2	10
77	Acetic anhydride at 100 K: the first crystal structure determination. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2016, 72, 753-757.	0.2	3
78	Reversible Dihydrogen Activation by Reduced Aryl Boranes as Main-Group Ambiphiles. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 14067-14071.	7.2	85
79	Platinum(0)-mediated C=O bond activation of ethers via an SN <sub>2</sub> mechanism. <i>Dalton Transactions</i> , 2016, 45, 18842-18850.	1.6	4
80	Trisodium citrate, Na <sub>3</sub> (C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> ). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 793-796.	0.2	15
81	Crystal structure, solvothermal synthesis, thermogravimetric studies and DFT calculations of a five-coordinate cobalt(II) compound based on the N,N-bis(2-hydroxyethyl)glycine anion. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 1463-1467.	0.2	2
82	Synthesis and structure of [NiL <sub>6</sub> ][B <sub>10</sub> H <sub>10</sub> ] (L = DMF or DMSO) as precursors for solid-phase synthesis of nickel(II) coordination compounds. <i>Inorganica Chimica Acta</i> , 2016, 451, 129-134.	1.2	17
83	Main group metal lone-pair- $\pi$ (arene) interactions: a new bonding mode for supramolecular associations. <i>CrystEngComm</i> , 2016, 18, 6960-6978.	1.3	30
84	Stabilisation of metastable polymorphs: the case of paracetamol form III. <i>Chemical Communications</i> , 2016, 52, 12028-12031.	2.2	39
85	$\pi$ -Hole Interactions Involving Nitro Compounds: Directionality of Nitrate Esters. <i>Crystal Growth and Design</i> , 2016, 16, 5520-5524.	1.4	67
86	Watson-Crick base pairing in 9-methyladenine and ethylene-9,9'-diadenine structures with close to 70% solvent content. <i>CrystEngComm</i> , 2016, 18, 6352-6357.	1.3	5
87	Peculiar Case of Levetiracetam and Etiracetam $\beta$ -Ketoglutaric Acid Cocrystals: Obtaining a Stable Conglomerate of Etiracetam. <i>Crystal Growth and Design</i> , 2016, 16, 5273-5282.	1.4	19
88	Getting the most out of PubChem for virtual screening. <i>Expert Opinion on Drug Discovery</i> , 2016, 11, 843-855.	2.5	98
89	Crystal Structure Determination of Dimenhydrinate after More than 60 Years: Solving Salt-Cocrystal Ambiguity via Solid-State Characterizations and Solubility Study. <i>Crystal Growth and Design</i> , 2016, 16, 5223-5229.	1.4	33
90	Stoichiometric and Nonstoichiometric Hydrates of Brucine. <i>Crystal Growth and Design</i> , 2016, 16, 6111-6121.	1.4	38



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91	Analysis of Oâ€“C, Sâ€“C and Oâ€“P angles: a database survey completed with four new X-ray crystal structures. <i>Structural Chemistry</i> , 2016, 27, 1831-1844.	1.0	9
92	Crystal structure of methyl 4-(4-hydroxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate monohydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 1335-1338.	0.2	3
93	Crystal growth and structural remarks on malonate-based lanthanide coordination polymers. <i>CrystEngComm</i> , 2016, 18, 7831-7842.	1.3	11
94	Octahedral molybdenum cluster complexes with aromatic sulfonate ligands. <i>Dalton Transactions</i> , 2016, 45, 15427-15435.	1.6	62
95	A ladder coordination polymer based on Ca <sup>2+</sup> and (4,5-dicyano-1,2-phenylene)bis(phosphonic acid): crystal structure and solution-state NMR study. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2016, 72, 685-691.	0.2	1
96	Crystal structure of bis(Î²-ethylene)Î³-pentamethylcyclopentadienyl)cobalt. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 1301-1304.	0.2	1
97	Concomitant polymorphs of 1,3-bis(3-fluorophenyl)urea. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2016, 72, 692-696.	0.2	7
98	Solvation and surface effects on polymorph stabilities at the nanoscale. <i>Chemical Science</i> , 2016, 7, 6617-6627.	3.7	128
99	The Hexahistidine Motif of Host-Defense Protein Human Calprotectin Contributes to Zinc Withholding and Its Functional Versatility. <i>Journal of the American Chemical Society</i> , 2016, 138, 12243-12251.	6.6	47
100	Synthesis, Electronic Spectroscopy, Cyclic Voltammetry, Photophysics, Electrical Properties and X-ray Molecular Structures of <i>meso</i> -Tetrakis[4-(benzoyloxy)phenyl]porphyrinato}zinc(II) Complexes with Aza Ligands. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 5004-5019.	1.0	24
101	Rhodium-Catalyzed Dehydrogenative Silylation of Acetophenone Derivatives: Formation of Silyl Enol Ethers versus Silyl Ethers. <i>Chemistry - A European Journal</i> , 2016, 22, 14717-14729.	1.7	21
102	Different molecular conformations co-exist in each of three 2-aryl-N-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)acetamides: hydrogen bonding in zero, one and two dimensions. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2016, 72, 664-669.	0.2	0
103	Probing Metal Ion Complexation of Ligands with Multiple Metal Binding Sites: The Case of Spiropyran. <i>Chemistry - A European Journal</i> , 2016, 22, 13976-13984.	1.7	36
104	X-ray Structures of 1-Ethynyl-2-Nitrobenzene and 1-Ethynyl-4,5-Dimethyl-2-Nitrobenzene: Correlation to the Enhanced Rate of Hydration and Investigation of the C-H...O Alkyne-Nitro Hydrogen Bonding. <i>Journal of Chemical Crystallography</i> , 2016, 46, 303-308.	0.5	1
105	Molecular packing preferences in $\alpha$ -bridge-flipped $\beta$ -isomeric aryl-2-pyridylhydrazones and 2-pyridinecarboxaldehyde arylhydrazones. <i>CrystEngComm</i> , 2016, 18, 7036-7048.	1.3	2
106	Now you see me too. <i>Science</i> , 2016, 353, 754-755.	6.0	1
107	<i>CrystalCMP</i> : an easy-to-use tool for fast comparison of molecular packing. <i>Journal of Applied Crystallography</i> , 2016, 49, 2172-2183.	1.9	72
108	Crystal structure of N,N <sup>2</sup> -bis[2-((benzyl){5-(dimethylamino)naphthalen-1-yl}sulfonyl)amino]ethyl)naphthalene-1,8:4,5-tetracarboximide 1,2-dichlorobenzene trisolvate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 1503-1508.	0.2	1

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109	A new solvate of furosemide with dimethylacetamide. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2016, 72, 997-1001.	0.2	1
110	Variation of the Molecular Conformation, Shape, and Cavity Size in Dinuclear Metalla-Macrocycles Containing Hetero-Ditopic Dithiocarbamate Carboxylate Ligands from a Homologous Series of N-Substituted Amino Acids. <i>Inorganic Chemistry</i> , 2016, 55, 12451-12469.	1.9	18
111	Beyond Rotatable Bond Counts: Capturing 3D Conformational Flexibility in a Single Descriptor. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 2347-2352.	2.5	30
112	Understanding the single-crystal-to-single-crystal solid-state phase transition of <i>dl</i> -methionine. <i>CrystEngComm</i> , 2016, 18, 9363-9373.	1.3	27
113	Solvates of selected fenamic acids with substituted pyridines: structure, thermal stability and desolvation. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 836-845.	0.5	6
114	Hydrogen-bonded network in the salt 4-methyl-1H-imidazol-3-ium picrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 772-775.	0.2	1
115	Structure of the Reduced Copper Active Site in Preprocessed Galactose Oxidase: Ligand Tuning for One-Electron O <sub>2</sub> Activation in Cofactor Biogenesis. <i>Journal of the American Chemical Society</i> , 2016, 138, 13219-13229.	6.6	35
116	Crystal Structures of New Lanthanide Hydroxybenzoates and Different Roles of LMCT State in the Excitation Energy Transfer to Eu <sup>3+</sup> Ions. <i>ChemistrySelect</i> , 2016, 1, 3428-3437.	0.7	12
117	Knowledge-Based Approaches to H-Bonding Patterns in Heterocycle-1-Carbohydrazoneamides. <i>Crystal Growth and Design</i> , 2016, 16, 6354-6362.	1.4	14
118	An insight into real and average structure from diffuse X-ray scattering – a case study. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 571-583.	0.5	4
119	Report on the sixth blind test of organic crystal structure prediction methods. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 439-459.	0.5	445
120	Self-assembly modes of glycyrrhetic acid esters in view of the crystal packing of related triterpene molecules. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 584-592.	0.5	7
121	Crystal structure prediction of rigid molecules. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 488-501.	0.5	6
122	Hydrothermal synthesis, structure, heterogeneous catalytic activity and photoluminescent properties of a novel homoleptic Sm(III)-organic framework. <i>Journal of Solid State Chemistry</i> , 2016, 244, 61-68.	1.4	21
123	Preferred Hydrogen-Bonding Partners of Cysteine: Implications for Regulating Cys Functions. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10288-10296.	1.2	57
124	High-pressure studies of three polymorphs of a palladium(II) oxathioether macrocyclic complex. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 357-371.	0.5	4
125	Capturing neon – the first experimental structure of neon trapped within a metal-organic environment. <i>Chemical Communications</i> , 2016, 52, 10048-10051.	2.2	13
126	It Isn't, It Is: The H...X (X = O, N, F, Cl) Interaction Really Is Significant in Crystal Packing. <i>Crystal Growth and Design</i> , 2016, 16, 4165-4168.	1.4	87



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127	Generation of crystal structures using known crystal structures as analogues. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 530-541.	0.5	18
128	Crystal structure of poly[N,N-diethyl-2-hydroxyethan-1-aminium [1/43-cyanido-1/3C:C:N-di-1/4-cyanido-1/4C:N-dicuprate(I)]]. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 892-896.	0.2	2
129	Crystal structure of methyl 1-allyl-4-methyl-1H-benzo[c][1,2]thiazine-3-carboxylate 2,2-dioxide. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1574-1576.	0.2	3
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593	Bis( $\lambda^2$ -{(E)-[(2E)-1,3-diphenylprop-2-en-1-ylidene]amino}-N-ethylcarbamidothioato- $\lambda^2$ N, $\lambda^2$ S)zinc(II): crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1001-1008.	0.2	7
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616	Crystal structure of 2-chloro-1,3-bis(2,6-diisopropylphenyl)-1,3,2-diazaphospholidine 2-oxide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017, 73, 735-737.	0.2	0
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620	Crystal structure of 4-[(3-methylbut-3-enoyl)oxy]phenyl 4-n-hexyloxybenzoate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017, 73, 1052-1055.	0.2	8
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625	A copper(II) paddle-wheel structure of tranexamic acid: dichloro-tetrakis[¼-4-(ammoniomethyl)cyclohexane-1-carboxylato-O,O']dicopper(II) dichloride hexahydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017, 73, 1421-1425.	0.2	3
626	Crystal structure of 3,3'-biisoxazole-5,5'-bis(methylene) dinitrate (BIDN). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017, 73, 644-646.	0.2	5
627	Crystal structure of 2-cyano-3,3-bis(ethylsulfanyl)- <i>N</i> - <i>o</i> -tolylacrylamide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017, 73, 752-754.	0.2	4
628	Crystal structures of two bicyclo[5.1.0]octanes: potassium <i>trans</i> -bicyclo[5.1.0]octane-4-carboxylate monohydrate and <i>cis</i> -bicyclo[5.1.0]octan-4-yl 4-bromobenzenesulfonate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017, 73, 1357-1362.	0.2	0
629	Oxidodiperoxidomolybdenum Complexes: Properties and Their Use as Catalysts in Green Oxidations. , 2017, , .		0
630	Crystal structure and DFT study of (<i>E</i>)-<i>N</i>-[2-(1<i>H</i>-indol-3-yl)ethyl]-1-(anthracen-9-yl)methanimine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017, 73, 1329-1332.	0.2	1

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631	Crystal structure of (2,2'-bipyridine- $\text{N}_2$ )bis(3,5-di- <i>tert</i> -butyl-o-benzoquinonato- $\text{O}_2$ )ruthenium(II). Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 459-462.	0.2	0
632	A dihydro- $\beta$ -agarofuran sesquiterpene from <i>Maytenus boaria</i> . Acta Crystallographica Section C, Structural Chemistry, 2017, 73, 451-457.	0.2	6
633	$\frac{1}{4}$ -Chlorido- $\frac{1}{4}$ -chlorido- $\frac{1}{3}$ -pyrrolidine-1-carbodithioato- $\frac{4}{3}$ - <i>S</i> : <i>S</i> , crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 720-725.	0.2	3
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635	Crystal structure of 5-O-benzoyl-2,3-O-isopropylidene-D-ribo-1,4-lactone. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 407-409.	0.2	0
636	Crystal structures of the Schiff base derivatives ( <i>E</i> )- <i>N</i> -(1 <i>H</i> -indol-3-yl)methylidene]isonicotinohydrazide ethanol monosolvate and ( <i>E</i> )- <i>N</i> -methyl-2-[1-(2-oxo-2 <i>H</i> -chromen-3-yl)ethylidene]hydrazinecarbothioamide. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 594-597.	0.2	4
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643	Crystal structure of dipotassium- <i>N</i> -carbodithioato- <i>L</i> -prolinate trihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1375-1378.	0.2	5
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651	Crystal structure of 4-amino-3-(thiophen-3-ylmethyl)-1H-1,2,4-triazole-5(4H)-thione. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1389-1392.	0.2	2
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655	Tris[( $\frac{1}{2}$ -methanolato)- $\frac{1}{4}$ -oxido-tris{[(E)-4-chloro-2-[[2-(pyridin-2-yl)ethyl]imino]methyl]phenolato}]manganese(III)) perchlorate $\cdot$ dichloromethane $\cdot$ diethyl ether (1/1.1/0.9). Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1113-1116.	0.2	4
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661	Crystal structure of chlorido(dimethyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 272 Td (sulfoxide- $\frac{1}{2}$ <i>S</i> )bis[4-(pyridin-2-yl)benzaldehyde] acetonitrile monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1279-1281.	0.2	2
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675	Crystal structure of phenyl-N-(3,5-dimethylphenyl)carbamate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 849-852.	0.2	0
676	Crystal structure of {(R)-N2-[(benzo[h]quinolin-2-yl)methyl]-N2'-[(benzo[h]quinolin-2-yl)methylidene]-1,1'-binaphthyl-2,2'-diamine- $\lambda^4$ N <sub>4</sub> N <sub>2</sub> Na <sub>2</sub> O <sub>2</sub> ·2CF <sub>3</sub> SO <sub>2</sub> Na·2CH <sub>2</sub> Cl <sub>2</sub> ·1.5H <sub>2</sub> O}·1.5CH <sub>2</sub> Cl <sub>2</sub> . Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 949-953.	0.2	0
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686	Three closely related 2-(2,3-dihydro-1,4-phenylene)bis[1-(methoxyphenyl)prop-2-en-1-ones]: supramolecular assemblies in one dimension mediated by hydrogen bonding and C-H...O interactions. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017, 73, 896-900.	0.2	3
687	Two closely related 2-(benzofuran-2-yl)-2-oxoethyl benzoates: structural differences and C-H...O hydrogen-bonded supramolecular assemblies. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017, 73, 1087-1091.	0.2	0
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756	Group 9 Metallacyclopentadienes as Key Intermediates in [2+2+2] Alkyne Cyclotrimerizations. Insight from Activation Strain Analyses. <i>ChemPhysChem</i> , 2018, 19, 1766-1773.	1.0	13
757	3-Methyl-1-[(E)-[1-(4-methylpyridin-2-yl)ethylidene]amino]thiourea: crystal structure and Hirshfeld surface analysis. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 256-260.	0.2	1



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761	Data-driven learning and prediction of inorganic crystal structures. <i>Faraday Discussions</i> , 2018, 211, 45-59.	1.6	66
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763	Evaluation of HER2-specific peptide ligand for its employment as radiolabeled imaging probe. <i>Scientific Reports</i> , 2018, 8, 2998.	1.6	22
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767	Protonation of inorganic 5-Fluorocytosine salts. <i>Journal of Molecular Structure</i> , 2018, 1161, 412-423.	1.8	1
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792	Crystal structure of the triethylammonium salt of 3-[(4-hydroxy-3-methoxyphenyl)(4-hydroxy-2-oxo-2- <i>H</i> -chromen-3-yl)methyl]-2-oxo-2- <i>H</i> -chromen-4-olate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 282-286.		2
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805	The ephemeral dihydrate of sulfanilic acid. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 7-12.	0.2	3
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808	Computational Design of a Photocontrolled Cytosine Deaminase. <i>Journal of the American Chemical Society</i> , 2018, 140, 14-17.	6.6	26
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828	Sulfur as hydrogen-bond acceptor in cocrystals of 2-thio-modified thymine. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 21-30.	0.2	4
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831	Complexes of Zn(II) and Cd(II) with 2-acetylpyridine -aminoguanidine " Syntheses, structures and DFT calculations. <i>Inorganica Chimica Acta</i> , 2018, 473, 160-168.	1.2	8
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849	<sup>79/81</sup> Br nuclear quadrupole resonance spectroscopic characterization of halogen bonds in supramolecular assemblies. <i>Chemical Science</i> , 2018, 9, 4555-4561.	3.7	22
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877	Molecular and supramolecular chemistry of mono- and di-selenium analogues of metal dithiocarbamates. <i>Coordination Chemistry Reviews</i> , 2018, 375, 410-423.	9.5	19
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1013	Synthesis, crystal structure and Hirshfeld surface analysis of tetraaquabis(isonicotinamide- <i>N</i> ) <i>Tj ETQq1</i> 1 0.784314 <i>rgBT /Ove</i> Communications, 2018, 74, 1026-1029.	0.2	1
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1024	Crystal structure of ( <i>Z</i> )-2-bromo-3-(3,5-di- <i>tert</i> -butyl-4-hydroxyphenyl)-1-phenylprop-2-en-1-one, C <sub>23</sub> H <sub>27</sub> BrO <sub>2</sub> . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2018, 233, 1019-1020.	0.1	9
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1051	Crystal structure of <i>N,N</i> -bis(2,4-difluorobenzoyloxy)benzene-1,2,4,5-tetracarboximide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 225-228.	0.2	0
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1055	Phosphoryl Podands Ph <sub>2</sub> P(O)CH <sub>2</sub> O(CH <sub>2</sub> CH <sub>2</sub> O) <sub>n</sub> CH <sub>2</sub> P(O)Ph <sub>2</sub> (Ln, n = 0-5): Complexation and Extraction of Rare Earth Elements. <i>Crystal Structures of [Ln<sub>2</sub>L<sub>03</sub>(NO<sub>3</sub>)<sub>6</sub>] · xH<sub>2</sub>O (Ln = Nd, x = 1.99; Ln = Eu, x = 1; Ln = Tm, x = 1.0784314) and [Ln<sub>2</sub>L<sub>03</sub>(NO<sub>3</sub>)<sub>6</sub>] · xH<sub>2</sub>O (Ln = Nd, x = 1.99; Ln = Eu, x = 1; Ln = Tm, x = 1.0784314)</i> , 2018, 63, 1372-1380.	0.3	4
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1106	Bismuth( <sup>iii</sup> )-thiophenedicarboxylates as host frameworks for lanthanide ions: synthesis, structural characterization, and photoluminescent behavior. <i>Dalton Transactions</i> , 2018, 47, 13419-13433.	1.6	13
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1121	Crystal structure, hydrogen bonding and Hirshfeld surface analysis of 2-amino-4-methoxy-6-methylpyrimidinium 4-chlorobenzoate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 656-659.	0.2	3
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1232	Structural study of mono-, di- and tetranuclear complexes of the {Re(CO) <sub>3</sub> } <sup>+</sup> fragment with thiosemicarbazone/thiosemicarbazone ligands containing benzothiazole or benzoxazole groups. <i>CrystEngComm</i> , 2018, 20, 4781-4792.	1.3	8

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1240	OChemDb: the free online Open Chemistry Database portal for searching and analysing crystal structure information. <i>Journal of Applied Crystallography</i> , 2018, 51, 1229-1236.	1.9	10
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1244	Spontaneous enantiomorphism in poly-phased alkaline salts of tris(oxalato)ferrate(III): crystal structure of cubic Na <sub>5</sub> [Fe(C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub> ] <sub>2</sub> . <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 905-909.	0.2	0
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1257	New Reactions for Old Ions: Cage Rearrangements, Hydrolysis, and Two-Electron Reduction of <i>nido</i> -Decaborane in Neat 1-Ethyl-3-Methylimidazolium Acetate. <i>ACS Omega</i> , 2018, 3, 8491-8496.	1.6	4
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1260	En Route to Chiral-at-Metal Ruthenium Complexes Containing Tripodal Tetradentate Ligands. <i>Organometallics</i> , 2018, 37, 3450-3464.	1.1	7
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1542	Counterion influence on dynamic spin properties in a V( <i>scpv</i> ) complex. <i>Chemical Science</i> , 2019, 10, 548-555.	3.7	23
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1555	Conformational analysis and potential anticancer activity of [Pt(phen)(L1- <i>S</i> ) <sub>2</sub> ] studied by single crystal X-ray diffraction and variable temperature <sup>1</sup> H and <sup>195</sup> Pt NMR spectroscopy. <i>New Journal of Chemistry</i> , 2019, 43, 3665-3672.	1.4	7
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1633	Structure and piezochromism of pyrene-1-carbaldehyde at high pressure. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 343-353.	0.5	7
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1639	Phosphanchalkogenide und ihre Metallkomplexe. V. Derivate von [2.2]Paracyclophanylphosphanen <sup>a</sup> . <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2019, 74, 389-404.	0.3	4
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1678	Metal-Organic Frameworks. <i>Green Energy and Technology</i> , 2019, , 137-172.	0.4	7
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1778	Coordination of 1-methyl-1,3-dihydro-2H-benzimidazole-2-selone to zinc and cadmium: Monotonic and non-monotonic bond length variations for $[H(\text{sebenzimMe})]_2MCl_2$ complexes ( $M = Zn, Cd, Hg$ ). <i>Polyhedron</i> , 2019, 164, 185-194.	1.0	3
1779	$Ba_3CrN_3H$ : A New Nitride-Hydride with Trigonal Planar $Cr^{4+}$ . <i>Inorganic Chemistry</i> , 2019, 58, 3302-3307.	1.9	16
1780	Electronic Structures of an $[Fe(NNR_2)]^{+0}$ Redox Series: Ligand Noninnocence and Implications for Catalytic Nitrogen Fixation. <i>Inorganic Chemistry</i> , 2019, 58, 3535-3549.	1.9	19
1781	Novel primary amide-based cationic metal complexes: green synthesis, crystal structures, Hirshfeld surface analysis and solvent-free cyanosilylation reaction. <i>Dalton Transactions</i> , 2019, 48, 3743-3757.	1.6	14
1782	The effective volumes of waters of crystallization: non-ionic pharmaceutical systems. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 784-787.	0.5	9
1783	Synthesis, Crystal Structure, and Hirshfeld Surface Analysis of Rubidium <i>trans</i> -Bis(N-methyliminodiacetato)chromate(III). <i>Crystallography Reports</i> , 2019, 64, 1011-1018.	0.1	1
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1788	Synthesis and structural characterization of the type-I clathrates $K_8Al_4Sn_4$ and $Rb_8Al_4Sn_4$ ( $a = 6.4 \text{ \AA}$ ). <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 1535-1540.	0.2	1
1789	Mechanochemical synthesis and X-ray structural characterization of three 3-nitrophenol cocrystals with three aminated cage azaadamantanes: the role of the stereoelectronic effect on intermolecular hydrogen-bonding patterns. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 1635-1643.	0.2	2
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1797	Tuning the Gate-Opening Pressure in a Switching pcu Coordination Network, X <sub>2</sub> pcu <sub>5</sub> Zn, by Pillar-Ligand Substitution. <i>Angewandte Chemie</i> , 2019, 131, 18380-18385.	1.6	12
1798	Balancing charge-transfer strength and triplet states for deep-blue thermally activated delayed fluorescence with an unconventional electron rich dibenzothiophene acceptor. <i>Journal of Materials Chemistry C</i> , 2019, 7, 13224-13234.	2.7	52
1799	Crystal structure of bromido-dimethyl-4-tolyl-(triphenylphosphine oxide)tin(IV), C <sub>27</sub> H <sub>28</sub> BrOPSn. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2019, 235, 163-165.	0.1	2
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1801	Hinged and Wide: A New P <sup>2</sup> P Ligand for Emissive [Cu(P <sup>2</sup> P)(N <sup>2</sup> N)][PF <sub>6</sub> ] Complexes. <i>Molecules</i> , 2019, 24, 3934.	1.7	10
1802	Computational screening of metal-organic frameworks for biogas purification. <i>Molecular Systems Design and Engineering</i> , 2019, 4, 1125-1135.	1.7	15
1803	Crystal structure of bis(di- <i>n</i> -butylammonium) tetrachloridodiphenylstannate(IV), C <sub>28</sub> H <sub>50</sub> Cl <sub>4</sub> N <sub>2</sub> Sn. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2019, 234, 889-891.	0.1	1
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1805	Singlet-Triplet Energy Gaps in Binuclear Copper Complexes and Organic Diradicals by Approximate Spin Projected Spin-unrestricted Coupled Cluster Method. <i>Chemistry Letters</i> , 2019, 48, 1441-1444.	0.7	3
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1808	Cyclometallated tridentate platinum(II) arylacetylide complexes: old wine in new bottles. <i>Chemical Society Reviews</i> , 2019, 48, 5547-5563.	18.7	111
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1826	Preparation and structure of 4-(dimethylamino)thiopivalophenone “intermolecular interactions in the crystal. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2019, 74, 825-831.	0.3	1
1828	Structural, Electrochemical, and Magnetic Studies of Bulky Uranium(III) and Uranium(IV) Metallocenes. <i>Inorganic Chemistry</i> , 2019, 58, 16629-16641.	1.9	28
1829	Metal-Free Deep Eutectic Solvents: Preparation, Physical Properties, and Significance. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7956-7964.	2.1	118
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1851	A collection of forcefield precursors for metal-organic frameworks. <i>RSC Advances</i> , 2019, 9, 36492-36507.	1.7	21
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1855	Perspective on computational simulations of glycosaminoglycans. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1388.	6.2	21
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1861	Crystal and Electron Properties of Carbamazepine-Aspirin Co-crystal. <i>Crystal Growth and Design</i> , 2019, 19, 1308-1321.	1.4	15
1862	The Preparation of Luminescent, Mechanochromic Molecular Containers from Non-Emissive Components: The Box Cations, [Au 6 (Triphos) 4 Br] 5+ and [Au 6 (Triphos) 4 Br 2 ] 4+. <i>Chemistry - A European Journal</i> , 2019, 25, 3849-3857.	1.7	8
1863	Coprocessing of Pharmaceutical Cocrystals for High Quality and Enhanced Physicochemical Stability. <i>Crystal Growth and Design</i> , 2019, 19, 876-888.	1.4	19
1864	Crystal structures of ammonium citrates. <i>Powder Diffraction</i> , 2019, 34, 35-43.	0.4	39
1865	Extrinsic Heavy Metal Atom Effect on the Solid-State Room Temperature Phosphorescence of Cyclic Triimidazole. <i>Chemistry - an Asian Journal</i> , 2019, 14, 853-858.	1.7	13
1866	Reactivity of homoleptic and heteroleptic core paddle wheel Cu(II) compounds. <i>Inorganica Chimica Acta</i> , 2019, 487, 295-306.	1.2	13



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1868	Self-Assembly of Aluminum- and Gallium-Based <i>meso</i> -Metallaporphyrins. Inorganic Chemistry, 2019, 58, 265-278.	1.9	3
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1879	Validation and Applications of Protein-Ligand Docking Approaches Improved for Metalloligands with Multiple Vacant Sites. Inorganic Chemistry, 2019, 58, 294-306.	1.9	35
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1886	Hypervalent organoselenium compounds stabilized by intramolecular coordination: synthesis and crystal structures. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 70-76.	0.2	3
1887	Two single-enantiomer amidophosphoesters: a database study on the chirality of (O) <sub>2</sub> P(O)(N)-based structures. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 77-84.	0.2	7
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1889	The Effect of $\beta$ -Hydrogen Atoms on Iron Speciation in Cross-Couplings with Simple Iron Salts and Alkyl Grignard Reagents. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 2769-2773.	7.2	41
1890	Incremental Introduction of Organocatalytic Activity into Conformationally Engineered Porphyrins. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 2448-2452.	1.2	19
1891	Succinic, fumaric, adipic and oxalic acid cocrystals of promethazine hydrochloride. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 107-119.	0.2	6
1892	Fluconazole: Synthesis and Structural Characterization of Four New Pharmaceutical Cocrystal Forms. <i>Crystal Growth and Design</i> , 2019, 19, 648-657.	1.4	30
1893	Fast and Accurate Uncertainty Estimation in Chemical Machine Learning. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 906-915.	2.3	102
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1897	In vitro anti-bacterial and time kill evaluation of binuclear tricyclohexylphosphanesilver(I) dithiocarbamates, {Cy <sub>3</sub> PAg(S <sub>2</sub> CNRR <sup>2</sup> ) <sub>2</sub> }. <i>Journal of Inorganic Biochemistry</i> , 2019, 192, 107-118.	1.5	19
1898	New chromium, molybdenum, and cobalt complexes of the chelating esp ligand. <i>Polyhedron</i> , 2019, 161, 93-103.	1.0	5
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1902	Significance of hydrogen bonding and other noncovalent interactions in determining octahedral tilting in the CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> hybrid organic-inorganic halide perovskite solar cell semiconductor. <i>Scientific Reports</i> , 2019, 9, 50.	1.6	95

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1903	Catalytic Metallopolymers from [2Fe $\mu$ S] Clusters: Artificial Metalloenzymes for Hydrogen Production. <i>Angewandte Chemie</i> , 2019, 131, 7617-7630.	1.6	42
1904	Assembly of Tetrazolylfuroxan Organic Salts: Multipurpose Green Energetic Materials with High Enthalpies of Formation and Excellent Detonation Performance. <i>Chemistry - A European Journal</i> , 2019, 25, 4225-4233.	1.7	60
1905	Quantifying API polymorphs in formulations using X-ray powder diffraction and multivariate standard addition method combined with net analyte signal analysis. <i>European Journal of Pharmaceutical Sciences</i> , 2019, 130, 36-43.	1.9	11
1906	A structural study of seven N-acylindolines and their Pd(II)-mediated intramolecular oxidative coupling reactions for the synthesis of pyrrolophenanthridone alkaloids. <i>Journal of Molecular Structure</i> , 2019, 1178, 341-351.	1.8	2
1907	Fully optimized implementation of the cluster $\mu$ molecule local correlation approach for electron correlation calculations of large systems. <i>Journal of Computational Chemistry</i> , 2019, 40, 1130-1140.	1.5	24
1908	On the influence of small chemical changes upon the supramolecular association in substituted 2-(phenoxy)-1,4-naphthoquinones. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2019, 234, 183-200.	0.4	1
1909	A novel binuclear hydrazone-based Cd(II) complex is a strong pro-apoptotic inducer with significant activity against 2D and 3D pancreatic cancer stem cells. <i>Journal of Inorganic Biochemistry</i> , 2019, 190, 45-66.	1.5	8
1910	A theoretical study of the bonding capabilities of the zinc $\mu$ zinc double bond. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25823.	1.0	5
1911	High-Pressure Structure and Properties of <i>N,N</i> -Dimethylformamide (DMF). <i>Crystal Growth and Design</i> , 2019, 19, 896-901.	1.4	8
1912	Chiral Discrete and Polymeric Uranyl Ion Complexes with (1 <i>R</i> ,3 <i>S</i> )-(+)-Camphorate Ligands: Counterion-Dependent Formation of a Hexanuclear Cage. <i>Inorganic Chemistry</i> , 2019, 58, 870-880.	1.9	22
1913	Chalcogen Bonding $\mu$ 2N Squares $\mu$ versus Competing Interactions: Exploring the Recognition Properties of Sulfur. <i>Chemistry - A European Journal</i> , 2019, 25, 323-333.	1.7	76
1914	Nonlinear optical organic $\mu$ inorganic crystals: synthesis, structural analysis and verification of harmonic generation in tri- <i>o</i> -chloroanilinium nitrate). <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2019, 75, 107-114.	0.0	6
1915	Nucleobase carbonyl groups are poor Mg <sup>2+</sup> inner-sphere binders but excellent monovalent ion binders $\mu$ a critical PDB survey. <i>Rna</i> , 2019, 25, 173-192.	1.6	31
1916	Toward Automated Tools for Characterization of Molecular Porosity. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 787-798.	2.3	3
1917	Exploring the Relationship between Intermolecular Interactions and Solid-State Photophysical Properties of Organic Co-Crystals. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9311-9322.	1.5	31
1918	Synthesis, structural investigations and pharmacological properties of a new zinc complex with a N4-donor Schiff base incorporating 2-pyridyl ring. <i>Inorganica Chimica Acta</i> , 2019, 487, 97-106.	1.2	12
1919	A Practical Guide to the Design of Molecular Crystals. <i>Crystal Growth and Design</i> , 2019, 19, 1426-1453.	1.4	222
1920	Converging a Knowledge-Based Scoring Function: DrugScore <sup>2018</sup> . <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 509-521.	2.5	48

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1922	Technology in the Service of Pedagogy: Teaching with Chemistry Databases. <i>Israel Journal of Chemistry</i> , 2019, 59, 572-582.	1.0	11
1923	Theophylline alkaloid as glue of paddle-wheel copper(II)-adenine entities to afford a rhomboid chain. <i>Inorganica Chimica Acta</i> , 2019, 484, 437-442.	1.2	5
1924	Synthesis, Structure and Nickel Carbonyl Complexes of Dialkylterphenyl Phosphines. <i>Chemistry - A European Journal</i> , 2019, 25, 260-272.	1.7	33
1925	Mono- and di-anionic coordination modes of arylazosalicylates in their bis( $\eta^5$ -cyclopentadienyl)titanium(IV) complexes: Syntheses and crystal structures. <i>Inorganica Chimica Acta</i> , 2019, 484, 469-480.	1.2	3
1926	<i>Chemoinformatics</i> , 2020, , 635-676.		2
1927	Polyhalogen- und Polyinterhalogen-Anionen von Fluor bis Iod. <i>Angewandte Chemie</i> , 2020, 132, 5506-5535.	1.6	24
1928	Polyhalogen and Polyinterhalogen Anions from Fluorine to Iodine. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 5464-5493.	7.2	79
1929	Role of N-terminus in function and dynamics of sirtuin 7: an <i>in silico</i> study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 1283-1291.	2.0	7
1930	Insights into the Structure of Halide-Rich Hydrochloric and Hydrobromic Acid: A Structural and Quantum-Chemical Investigation of the $[H_6X_4O_2]^{2-}$ ( $X = Cl, Br$ ) Anions. <i>Journal of Chemical Crystallography</i> , 2020, 50, 69-76.	0.5	1
1931	Growth and characterization of a new chlorine substituted chalcone: A third order nonlinear optical material. <i>Journal of Molecular Structure</i> , 2020, 1201, 127137.	1.8	10
1932	Synthesis, characterization and DFT studies of 6-bis(2-(thiazol-4-yl)-benzimidazol-1-yl)hexane hemihydrate crystal: Experimental and theoretical investigation. <i>Journal of Molecular Structure</i> , 2020, 1202, 127253.	1.8	7
1933	Autonomous Discovery in the Chemical Sciences Part II: Outlook. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 23414-23436.	7.2	139
1934	Magnetic properties of calixarene-supported metal coordination clusters. <i>Coordination Chemistry Reviews</i> , 2020, 402, 213066.	9.5	32
1935	Halogen interactions in dinuclear copper(II) 2,4-dibromophenoxyacetate crystal structure and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2020, 1202, 127227.	1.8	5
1936	Enumeration of <i>de novo</i> inorganic complexes for chemical discovery and machine learning. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 139-152.	1.7	23
1937	A sustainable peroxophosphomolybdate/H <sub>2</sub> O <sub>2</sub> system for the oxidative removal of organosulfur compounds from simulated and real high-sulfur diesels. <i>Applied Catalysis A: General</i> , 2020, 589, 117154.	2.2	19
1938	Evaluation of nanocellulose interaction with water pollutants using nanocellulose colloidal probes and molecular dynamic simulations. <i>Carbohydrate Polymers</i> , 2020, 229, 115510.	5.1	24

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1939	Relationships between Anhydrous and Solvated Species of Dexketoprofen Trometamol: A Solid-State Point of View. <i>Crystal Growth and Design</i> , 2020, 20, 226-236.	1.4	11
1940	ImageDataExtractor: A Tool To Extract and Quantify Data from Microscopy Images. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2492-2509.	2.5	29
1941	Terbium metal organic framework: Microwave synthesis and selective sensing of nitrite. <i>Inorganic Chemistry Communication</i> , 2020, 111, 107627.	1.8	11
1942	Ligand-Assisted Volatilization and Thermal Stability of Bis(imido)dichloromolybdenum(VI) ( $[(t\text{-BuN}^{\ominus})_2\text{MoCl}_2]_2$ ) and Its Adducts. <i>Organometallics</i> , 2020, 39, 916-927.	1.1	16
1943	Heterometallic Copper-Vanadium Compounds: Crystal Structures of Polymers $[\text{Cu}(\text{im})_4(\text{V}_2\text{O}_4(\text{mand})_2)]_n$ and $[\text{Cu}(\text{im})_4(\text{V}_2\text{O}_4((\text{S})\text{-mand})_2)]_n \cdot 2n\text{H}_2\text{O}$ (imidazole, mandelato). <i>Journal of Chemical Crystallography</i> , 2020, 50, 373-380.	0.5	0
1944	Spin-crossover behavior of bis[dihydrobis(4-methylpyrazol-1-yl-borate)]-(2,2'-bipyridine)iron and analogous complexes in the bulk and in thin films: Elucidating the influence of $\pi$ - $\pi$ -interactions on the type of spin transition. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 094001.	0.7	4
1945	Evidence for Non-Innocence of a $\text{D}^2$ -Diketonate Ligand. <i>Chemistry - A European Journal</i> , 2020, 26, 2143-2147.	1.7	9
1946	Autonome Entdeckung in den chemischen Wissenschaften, Teil II: Ausblick. <i>Angewandte Chemie</i> , 2020, 132, 23620-23643.	1.6	4
1947	Halogen versus Hydrogen Bonding in Binary Cocrystals: Novel Conformation a Coformer with [2+2] Photoreactivity of Criss-Crossed C=C Bonds. <i>ChemPhysChem</i> , 2020, 21, 154-163.	1.0	15
1948	A combined experimental and computational study of a supramolecular assembly based on cationic zinc(II)-ethanesulfonate. <i>Journal of Molecular Structure</i> , 2020, 1202, 127206.	1.8	1
1949	Supramolecular assembly of a 2D coordination polymer bearing pyridine-N-oxide-2,5-dicarboxylic acid and copper ion: X-ray crystallography and DFT calculations. <i>Journal of Molecular Structure</i> , 2020, 1202, 127243.	1.8	22
1950	Syntheses and electron density distribution studies in two new imidazole derivatives. <i>Journal of Molecular Structure</i> , 2020, 1206, 127657.	1.8	5
1951	Coordinating Ability of Anions, Solvents, Amino Acids, and Gases towards Alkaline and Alkaline-Earth Elements, Transition Metals, and Lanthanides. <i>Chemistry - A European Journal</i> , 2020, 26, 4350-4377.	1.7	67
1952	Cooperative Strong Charge-Assisted $\text{H}^{\ominus}\text{A}\cdots\text{O}$ Hydrogen Bonding and Weaker Nonconventional $\text{C}^{\ominus}\text{H}\cdots\text{N}$ Hydrogen Bonding in the Formation of Extended Hydrogen-Bonded Networks with 2,3,5,6-Tetrafluorobenzoic Acid. <i>Crystal Growth and Design</i> , 2020, 20, 1565-1571.	1.4	5
1953	Overcoming Crystallinity Limitations of Aluminium Metal-Organic Frameworks by Oxalic Acid Modulated Synthesis. <i>Chemistry - A European Journal</i> , 2020, 26, 3564-3570.	1.7	14
1954	Halogen- $\text{C}_2\text{H}_2$ Binding in Ultramicroporous Metal-Organic Frameworks (MOFs) for Benchmark $\text{C}_2\text{H}_2/\text{CO}_2$ Separation Selectivity. <i>Chemistry - A European Journal</i> , 2020, 26, 4923-4929.	1.7	72
1955	Revisiting van der Waals Radii: From Comprehensive Structural Analysis to Knowledge-Based Classification of Interatomic Contacts. <i>ChemPhysChem</i> , 2020, 21, 370-376.	1.0	39
1956	<code>fromage</code> : A library for the study of molecular crystal excited states at the aggregate scale. <i>Journal of Computational Chemistry</i> , 2020, 41, 1045-1058.	1.5	24

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1957	Triel bond and coordination of triel centres – Comparison with hydrogen bond interaction. <i>Coordination Chemistry Reviews</i> , 2020, 407, 213171.	9.5	72
1958	Cu(II) coordination to His-containing linear peptides and related branched ones: Equalities and diversities. <i>Journal of Inorganic Biochemistry</i> , 2020, 205, 110980.	1.5	8
1959	Hydroperoxo double hydrogen bonding: stabilization of hydroperoxo complexes exemplified by triphenylsilicon and triphenylgermanium hydroperoxides. <i>CrystEngComm</i> , 2020, 22, 1922-1928.	1.3	6
1960	Formation of a four-bladed waterwheel-type chloro-bridged dicopper(II) complex with dithiamacrocyclic double exo-coordination. <i>Dalton Transactions</i> , 2020, 49, 1365-1369.	1.6	3
1961	IMPRESSION – prediction of NMR parameters for 3-dimensional chemical structures using machine learning with near quantum chemical accuracy. <i>Chemical Science</i> , 2020, 11, 508-515.	3.7	66
1962	C-H...N hydrogen bonding in an overlayer of s-triazine physisorbed on a graphite surface. <i>Molecular Physics</i> , 2020, 118, e1706777.	0.8	4
1963	A Co-MOF with a (4,4)-connected binodal two-dimensional topology: synthesis, structure and photocatalytic properties. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 23-29.	0.2	8
1964	Influence of counterions on the supramolecular frameworks of isoquinoline-based silver(I) complexes. <i>CrystEngComm</i> , 2020, 22, 95-104.	1.3	0
1965	Structural characterization and magnetic property studies of a mixed-valence {CoIII CoII4} complex with a 1/4-oxo tetrahedral {CoII4} motif. <i>Dalton Transactions</i> , 2020, 49, 932-940.	1.6	4
1966	The solid-state structures and ligand cavity evaluation of lanthanide(III) complexes of a DOTA analogue with a (dibenzylamino)methylphosphinate pendant arm. <i>Dalton Transactions</i> , 2020, 49, 1555-1569.	1.6	4
1967	Zero-, mono- and diperic uranyl ion complexes with the diphenate dianion: influences of transition metal ion coordination and differential U(VI) chelation. <i>Dalton Transactions</i> , 2020, 49, 817-828.	1.6	10
1968	Two New Coordination Polymers with UO <sub>2</sub> <sup>2+</sup> Units and Fluorinated Aromatic Carboxylate Linkers. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2020, 646, 156-161.	0.6	2
1969	Synthesis and structural characterizations of novel atropisomeric ferrocene-containing six-membered cyclic ureas. <i>Polyhedron</i> , 2020, 177, 114316.	1.0	8
1970	Mechanochemical Formation and –Disappearance– of Caffeine – Citric-Acid Cocrystal Polymorphs. <i>Crystal Growth and Design</i> , 2020, 20, 1119-1129.	1.4	13
1971	In Silico Investigation into H <sub>2</sub> Uptake in MOFs: Combined Text/Data Mining and Structural Calculations. <i>Langmuir</i> , 2020, 36, 119-129.	1.6	6
1972	Does repeat synthesis in materials chemistry obey a power law?. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 877-882.	3.3	38
1973	Computer-aided drug design of small molecule inhibitors of the ERCC1-XPF protein – protein interaction. <i>Chemical Biology and Drug Design</i> , 2020, 95, 460-471.	1.5	15
1974	Hierarchy of Intermolecular Interactions and Selective Topochemical Reactivity in Different Polymorphs of Fused-Ring Heteroaromatics. <i>Crystal Growth and Design</i> , 2020, 20, 1229-1236.	1.4	13



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1975	How Chemical Environment Activates Anthralin and Molecular Oxygen for Direct Reaction. <i>Journal of Organic Chemistry</i> , 2020, 85, 1315-1321.	1.7	2
1976	Anion mediated switching from mono- to polymer structure in copper(II) complexes with 4,6-dimethylpyrimidinylhydrazone 1-phenyl-3-methyl-4-formylpyrazol-5-one. <i>Inorganica Chimica Acta</i> , 2020, 502, 119284.	1.2	1
1977	Structural peculiarities and luminescence of europium dipivaloylmethanates with 2,2'-bipyridine derivatives. Polymorphism of [Eu(DPM)3Bpy]. <i>Inorganica Chimica Acta</i> , 2020, 502, 119294.	1.2	6
1978	Comparison of induction methods for supersaturation: pH shift versus solvent shift. <i>International Journal of Pharmaceutics</i> , 2020, 573, 118862.	2.6	6
1979	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. <i>Journal of Inorganic Biochemistry</i> , 2020, 203, 110930.	1.5	19
1980	Crystal Structures of Missing Links in the Early History of Solid-State Reactions: The Group IA Acrylates and Methacrylates. <i>Crystal Growth and Design</i> , 2020, 20, 330-336.	1.4	4
1981	Bis(2,1,3-benzotelluradiazolidyl)2,1,3-benzotelluradiazole: a pair of radical anions coupled by Te-N chalcogen bonding. <i>Chemical Communications</i> , 2020, 56, 1113-1116.	2.2	18
1982	Metal-organic architectures driven by a multifunctional 6-aminouracil spacer: structures, noncovalent interactions, and conductivity. <i>CrystEngComm</i> , 2020, 22, 829-840.	1.3	7
1983	Prediction of correct intermolecular interactions in host-guest systems involving cyclodextrins. <i>Journal of Molecular Structure</i> , 2020, 1205, 127517.	1.8	6
1984	Phosphorescent heteroleptic iridium(III) cyclometallates: Improved syntheses of acetylacetonate complexes and quantum chemical studies of their excited state properties. <i>Polyhedron</i> , 2020, 176, 114256.	1.0	4
1985	Assessing the Role of Metal Identity on CO <sub>2</sub> Adsorption in MOFs Containing M-OH Functional Groups. <i>Chemistry of Materials</i> , 2020, 32, 489-497.	3.2	50
1986	Understanding the Separation Mechanism of C <sub>2</sub> H <sub>6</sub> /C <sub>2</sub> H <sub>4</sub> on Zeolitic Imidazolate Framework ZIF-7 by Periodic DFT Investigations. <i>Journal of Physical Chemistry C</i> , 2020, 124, 256-266.	1.5	9
1987	New $\beta$ -unsubstituted isoxazolones as potent human neutrophil elastase inhibitors: Synthesis and molecular dynamic simulation. <i>Drug Development Research</i> , 2020, 81, 338-349.	1.4	11
1988	Synthesis and biological evaluation of fluorescent GAT-ligands based on meso-substituted BODIPY dyes. <i>Medicinal Chemistry Research</i> , 2020, 29, 301-327.	1.1	4
1989	Trapped Intermediate of a Meerwein-Ponndorf-Verley Reduction of Hydroxy Benzaldehyde to a Dialkoxide by Titanium Alkoxides. <i>Inorganic Chemistry</i> , 2020, 59, 880-890.	1.9	2
1990	Interplay between Ionization and Tautomerism in Bioactive $\beta$ -Enamino Ester-Containing Cyclic Compounds: Study of Annulated 1,2,3,6-Tetrahydroazocine Derivatives. <i>Journal of Physical Chemistry B</i> , 2020, 124, 28-37.	1.2	3
1991	Phase behaviour and heat capacities of selected 1-ethyl-3-methylimidazolium-based ionic liquids. <i>Journal of Chemical Thermodynamics</i> , 2020, 142, 106020.	1.0	26
1992	Conformation-dependent restraints for polynucleotides: the sugar moiety. <i>Nucleic Acids Research</i> , 2020, 48, 962-973.	6.5	16

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1994	Flat or angular? The impact of the nitrogen atom hybridization on the docking results for arylpiperazine derivatives as an example. <i>Structural Chemistry</i> , 2020, 31, 823-829.	1.0	1
1995	Efficient Screening for Ternary Molecular Ionic Cocrystals Using a Complementary Mechanosynthesis and Computational Structure Prediction Approach. <i>Chemistry - A European Journal</i> , 2020, 26, 4752-4765.	1.7	27
1996	Synthesis of Highly Fluorinated Arene Complexes of [Rh(Chelating Phosphine)] <sup>+</sup> Cations, and their use in Synthesis and Catalysis. <i>Chemistry - A European Journal</i> , 2020, 26, 2883-2889.	1.7	9
1997	A structural and spectroscopic overview of molecular lanthanide complexes with fluorinated O-donor ligands. <i>Coordination Chemistry Reviews</i> , 2020, 404, 213098.	9.5	17
1998	The prediction of far-infrared spectra for molecular crystals of forensic interest â€“ Phenylethylamine, ephedrine & pseudoephedrine. <i>Forensic Chemistry</i> , 2020, 17, 100204.	1.7	2
1999	Combining Embedded Mean-Field Theory with Linear-Scaling Density-Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 354-365.	2.3	3
2000	Crystal structure of bisoprolol fumarate Form I, (C <sub>18</sub> H <sub>32</sub> NO <sub>4</sub> ) (C <sub>4</sub> H <sub>2</sub> O <sub>4</sub> ) <sub>0.5</sub> . <i>Powder Diffraction</i> , 2020, 35, 34-40.	0.4	1
2001	An Adaptable Nâ€Heterocyclic Carbene Macrocycle Hosting Copper in Three Oxidation States. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 5696-5705.	7.2	27
2002	Theoretical studies of perimidine and its derivatives: structures, energies, and spectra. <i>Structural Chemistry</i> , 2020, 31, 25-35.	1.0	4
2003	An overview on trace CO <sub>2</sub> removal by advanced physisorbent materials. <i>Journal of Environmental Management</i> , 2020, 255, 109874.	3.8	45
2004	Theoretical modeling of the chemical synthesis and detonation performance of polynitrocubane derivatives. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26117.	1.0	2
2005	Atomistic simulations of Epoxy/Water/Aluminum systems using the ReaxFF method. <i>Computational Materials Science</i> , 2020, 173, 109424.	1.4	8
2006	Ionic liquids based on 1-ethyl-3-methylimidazolium cation and anions of tetrafluoroborate and bis(trifluoromethylsulfonyl)imide: Structural and thermodynamic properties by DFT study. <i>Journal of Molecular Liquids</i> , 2020, 299, 112209.	2.3	8
2007	[3+2] Cycloaddition of diaryldiazomethanes with (E)-3,3,3-trichloro-1-nitroprop-1-ene: An experimental, theoretical and structural study. <i>Journal of Molecular Structure</i> , 2020, 1203, 127473.	1.8	20
2008	High-pressure behavior of the crystal structure of the fullerene molecular complex with ferrocene C <sub>60</sub> ·[Fe(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> ] <sub>2</sub> . <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2020, 28, 295-298.	1.0	2
2009	Capsaicin Is a Negative Allosteric Modulator of the 5-HT <sub>3</sub> Receptor. <i>Frontiers in Pharmacology</i> , 2020, 11, 1274.	1.6	7
2010	Tetrel Bonding Interactions Involving Carbon at Work: Recent Advances in Crystal Engineering and Catalysis. <i>Journal of Carbon Research</i> , 2020, 6, 60.	1.4	12

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2011	Computer-aided drug design against spike glycoprotein of SARS-CoV-2 to aid COVID-19 treatment. <i>Heliyon</i> , 2020, 6, e05278.	1.4	20
2012	Six transition metal-organic materials with the ditopic 4,4'-diaminodiphenylmethane ligand: Synthesis, structure characterization and luminescent properties. <i>Polyhedron</i> , 2020, 192, 114844.	1.0	3
2013	Mapping out the Relative Influence of Hydrogen and Halogen Bonds in Crystal Structures of a Family of Amide-Substituted Pyridines. <i>Crystal Growth and Design</i> , 2020, 20, 7399-7410.	1.4	10
2014	Visible light driven generation and alkyne insertion reactions of stable bis-cyclometalated Pt( $\sigma$ -C <sub>3</sub> H <sub>3</sub> ) hydrides. <i>Chemical Science</i> , 2020, 11, 12095-12102.	3.7	9
2015	Refinement of organic crystal structures with multipolar electron scattering factors. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2020, 76, 92-109.	0.0	20
2016	Machine learning for halide perovskite materials. <i>Nano Energy</i> , 2020, 78, 105380.	8.2	65
2017	New members of the polynuclear manganese family: MnII <sub>2</sub> MnIII <sub>2</sub> single-molecule magnets and MnIII <sub>3</sub> MnIII <sub>8</sub> antiferromagnetic complexes. Synthesis and magnetostructural correlations. <i>Dalton Transactions</i> , 2020, 49, 13970-13985.	1.6	6
2018	f-Element silicon and heavy tetrel chemistry. <i>Chemical Science</i> , 2020, 11, 10871-10886.	3.7	21
2019	Comprehensive Protocol for the Identification and Characterization of New Psychoactive Substances in the Service of Law Enforcement Agencies. <i>Frontiers in Chemistry</i> , 2020, 8, 693.	1.8	6
2020	Intramolecular Spodium Bonds in Zn(II) Complexes: Insights from Theory and Experiment. <i>International Journal of Molecular Sciences</i> , 2020, 21, 7091.	1.8	41
2021	Aperiodic metal-organic frameworks. <i>Chemical Science</i> , 2020, 11, 11094-11103.	3.7	11
2022	Ligand effects on the dimensionality of cyclophosphazene-based mercury(II) coordination polymers: Structures, UV-Visible absorption and thermal properties. <i>Polyhedron</i> , 2020, 192, 114823.	1.0	9
2023	Synchrotron far-infrared spectra for the characterisation of molecular crystals of forensic interest: Amphetamine, methamphetamine, MDA, MDMA and substituted methcathinones. <i>Vibrational Spectroscopy</i> , 2020, 110, 103115.	1.2	2
2024	Polymer structure and property effects on solid dispersions with haloperidol: Poly(N-vinyl) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50	2.6	18
2025	Identification of Noncompetitive Protein-Ligand Interactions for Structural Optimization. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 6595-6611.	2.5	10
2026	Rivalry between Regium and Hydrogen Bonds Established within Diatomic Coinage Molecules and Lewis Acids/Bases. <i>ChemPhysChem</i> , 2020, 21, 2557-2563.	1.0	11
2027	Understanding the geometric diversity of inorganic and hybrid frameworks through structural coarse-graining. <i>Chemical Science</i> , 2020, 11, 12580-12587.	3.7	13
2028	Crystallization of chiral molecular compounds: what can be learned from the Cambridge Structural Database?. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2020, 76, 307-315.	0.5	34

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2438	Crystal structures and temperature-dependent photoluminescence of lanthanide coordination frameworks of mixed-benzenedicarboxylates. <i>Journal of Coordination Chemistry</i> , 2020, 73, 333-345.	0.8	3
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2768	Crystal structure of tofacitinib dihydrogen citrate (Xeljanz <sup>®</sup> ), (C <sub>16</sub> H <sub>21</sub> N <sub>6</sub> O)(H <sub>2</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> ). <i>Powder Diffraction</i> , 2021, 36, 92-99.		0
2769	Crystal structures of zinc(II) complexes with $\hat{I}^2$ -hydroxypyridinecarboxylate ligands: examples of structure-directing effects used in inorganic crystal engineering. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 193-204.	0.5	2
2770	G-RMSD: Root Mean Square Deviation Based Method for Three-Dimensional Molecular Similarity Determination. <i>Bulletin of the Chemical Society of Japan</i> , 2021, 94, 655-665.	2.0	13
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2772	The Impact of Halogen Substituents on the Synthesis and Structure of Co-Crystals of Pyridine Amides. <i>Molecules</i> , 2021, 26, 1147.	1.7	4
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2779	Crystal structure of a methanol solvate of a macrocycle bearing two flexible side-arms. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 233-236.	0.2	3
2780	Crystal structure of ( <i>E</i> )-doxepin hydrochloride, C <sub>19</sub> H <sub>22</sub> NOCl. <i>Powder Diffraction</i> , 2021, 36, 43-49.	0.4	1
2781	Crystal structure and Hirshfeld surface analysis of ( <i>S</i> )-3-hydroxy-2-[(3 <i>S</i> ,6 <i>S</i> ,7 <i>S</i> )-(4-methylphenylsulfonyl)-2,3,3a,6,7,7a-hexahydro-2 <i>H</i> -3a,6-epoxy-1 <i>H</i> -indole-3-carboxylate]nickel(II) tetrapotassium] 4.8-hydrate]. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 260-265.		
2782	Crystal structure and Hirshfeld surface analysis of poly[[bis[1,4-dioxane-2,5-diy]bis(carbamoylmethanoato)]nickel(II) tetrapotassium] 4.8-hydrate]. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 298-304.		
2783	Crystal structure of pimecrolimus Form B, C <sub>43</sub> H <sub>68</sub> ClNO <sub>11</sub> . <i>Powder Diffraction</i> , 2021, 36, 35-42.	0.4	0
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2785	Multigram Preparation of BRD4780 Enantiomers and Assignment of Absolute Stereochemistry. <i>Journal of Organic Chemistry</i> , 2021, 86, 4281-4289.	1.7	2
2786	Molecular cannibalism: Sacrificial materials as precursors for hollow and multidomain single crystals. <i>Nature Communications</i> , 2021, 12, 957.	5.8	15
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2789	Crystal structure of pomalidomide Form I, C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub> . <i>Powder Diffraction</i> , 2021, 36, 114-119.	0.4	1
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2791	Accurate prediction of terahertz spectra of molecular crystals of fentanyl and its analogs. <i>Scientific Reports</i> , 2021, 11, 4062.	1.6	8

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2793	AFLOW-XtalFinder: a reliable choice to identify crystalline prototypes. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	28
2794	Structural and theoretical analysis of 2-chloro-4-nitroaniline and 2-methyl-6-nitroaniline salts. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 125-136.	0.2	0
2795	Crystal structure of $\text{cis}-(1,4,8,11\text{-tetraazacyclotetradecane-}\hat{\rho}\text{-}4)$ $\text{Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 627}$ <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 222-225.	0.2	0
2796	Synthesis and Characterization of Photoactive Methyl 4-Bromo-3-((2,6-Difluorophenyl)diazanyl) Benzoate. <i>Journal of Chemical Crystallography</i> , 2021, 51, 582.	0.5	0
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2799	Crystal structure of 2-[( <i>E</i> )-2-(4-bromophenyl)diazene-1-yl]-4,5-bis(4-methoxyphenyl)-1 <i>H</i> -imidazole: the first example of a structurally characterized triarylazoimidazole. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 305-308.	0.2	2
2800	Crystal structure of edoxaban tosylate monohydrate Form I, $(\text{C}_{24}\text{H}_{31}\text{ClN}_7\text{O}_4\text{S})(\text{C}_7\text{H}_7\text{O}_3\text{S})(\text{H}_2\text{O})$ . <i>Powder Diffraction</i> , 2021, 36, 107-113.	0.4	1
2801	Intermolecular Interactions between Thiocyanato Ligands in Metal Complexes. <i>Crystal Growth and Design</i> , 2021, 21, 1636-1644.	1.4	4
2802	Quantum Chemical Modeling of Mechanical Properties of Aspirin Polymorphic Modifications. <i>Crystal Growth and Design</i> , 2021, 21, 2176-2186.	1.4	10
2803	Crystal structure and Hirshfeld surface analysis of 2-benzyl-4,5-dibromo-2,3,3a,4,5,6,7,7a-octahydro-3a,6-epoxy-1 <i>H</i> -isoindol-1-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 255-259.	0.2	3
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2805	Synthesis and characterization of enantiopure planar-chiral phosphorus-linked diferrocenes. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 152-160.	0.2	0
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2807	Structural investigation of <i>N</i> -[2-(4-fluoro-3-phenoxybenzoyl)hydrazinecarbothiyl]benzamide and <i>N</i> -[2-(4-fluoro-3-phenoxybenzoyl)hydrazinecarbothiyl]-4-methoxybenzamide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 277-281.	0.2	0
2808	2-Amino-4-(4-chloro-1-ethyl-2,2-dioxo-1 <i>H</i> -benzo[ <i>c</i> ][1,2]thiazin-3-yl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4 <i>H</i> -chromene single-crystal X-ray diffraction study and Hirshfeld surface analysis. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 294-297.	0.2	0
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2825	Synthesis and crystal structure of <i>catena</i> -poly[[tetra- $\frac{1}{4}$ -acetato-copper(II)]- $\frac{1}{4}$ -6-ethoxy- <i>N</i> - <sup>2</sup> , <i>N</i> - <sup>4</sup> -bis[2-(pyridin-2-yl)ethyl]-1,3,5-triazine-2,4-diamine]. Acta Crystallographica Section E: Crystallographic Communications, 2021, 77, 319-323.	0.2	0
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2831	Crystal structure of tamsulosin hydrochloride, C <sub>20</sub> H <sub>29</sub> N <sub>2</sub> O <sub>5</sub> SCl. <i>Powder Diffraction</i> , 2021, 36, 85-91.	0.4	1
2832	Crystal structure and Hirshfeld surface analysis of ethyl 2-[9-(2-hydroxyphenyl)-3,3,6,6-tetramethyl-1,8-dioxo-2,3,4,4a,5,6,7,8a,9,9a,10,10a-dodecahydroacridin-10-yl]acetate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 247-250.		1
2833	Crystal structure of tezacaftor Form A, C <sub>26</sub> H <sub>27</sub> F <sub>3</sub> N <sub>2</sub> O <sub>6</sub> . <i>Powder Diffraction</i> , 2021, 36, 56-62.	0.4	0
2834	Large-Scale Analysis of Bioactive Ligand Conformational Strain Energy by <i>Ab Initio</i> Calculation. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1180-1192.	2.5	16
2835	Heteroleptic [Cu(P <sup>∧</sup> P)(N <sup>∧</sup> N)][PF <sub>6</sub> ] Complexes: Effects of Isomer Switching from 2,2'-biquinoline to 1,1'-biisoquinoline. <i>Crystals</i> , 2021, 11, 185.	1.0	5
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2848	Computational Identification of Connected MOF@COF Materials. <i>Journal of Physical Chemistry C</i> , 2021, 125, 5897-5903.	1.5	12
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2850	Crystal structure of (<i>E</i>)-1-(3-benzyl-5-phenyl-1,3-thiazol-2-ylidene)-2-[(<i>E</i>)-1,2,3,4-tetrahydronaphthalen-1-ylidene]hydrazin<sub>2</sub>ium bromide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 420-423.		0
2851	The crystal structures, Hirshfeld surface analyses and energy frameworks of 8-[1-[3-(cyclopent-1-en-1-yl)benzyl]piperidin-4-yl]-2-methoxyquinoline and 8-[4-[3-(cyclopent-1-en-1-yl)benzyl]piperazin-1-yl]-2-methoxyquinoline. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 372-377.	0.2	0
2852	Crystal structure of <i>tert</i>-butyl 4-[4-(4-fluorophenyl)-2-methylbut-3-yn-2-yl]piperazine-1-carboxylate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 360-365.	0.2	1
2853	Crystal structures of 1-(4-chlorophenyl)-4-(4-methylphenyl)-2,5-dioxo-1,2,5,6,7,8-hexahydroquinoline-3-carboxylic acid and 4-(4-methoxyphenyl)-1-(4-methylphenyl)-2,5-dioxo-1,2,5,6,7,8-hexahydroquinoline-3-carbonitrile. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 351-355.	0.2	1
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2862	ParaMol: A Package for Automatic Parameterization of Molecular Mechanics Force Fields. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2026-2047.	2.5	22
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2866	An electrochemical and computational chemistry study of substituted benzophenones. <i>Electrochimica Acta</i> , 2021, 373, 137894.	2.6	18
2867	Synthesis, Characterization, and Solid-State Structural Chemistry of Uranium(IV) Aliphatic Dicarboxylates. <i>Crystal Growth and Design</i> , 2021, 21, 2429-2444.	1.4	2
2868	Crystallographic characterization of $(C_5H_4SiMe_3)_3U(BH_4)_4$ . <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 383-389.	0.2	0
2869	Synthesis and structure of a complex of copper(I) with <i>L</i> -cysteine and chloride ions containing $Cu_{12}S_6$ nanoclusters. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 324-330.	0.2	3
2870	Crystal structure and Hirshfeld surface analysis of $(3S,3aR,6aS)-3-(1,3-diphenyl-1H-pyrazol-4-yl)-5-(4-methoxyphenyl)-2-phenyl-3,3a,4,5,6,6a-hexahydro-2H$ . <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 356-359.		
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2872	Crystal structure of eltrombopag olamine Form I, $(C_2H_8NO)_2(C_25H_{20}N_4O_4)$ . <i>Powder Diffraction</i> , 2021, 36, 100-106.	0.4	1
2873	Crystal structure and Hirshfeld surface analysis of $(Z)-3-methyl-4-(thiophen-2-ylmethylidene)isoxazol-5(4H)-one$ . <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 378-382.	0.2	0
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2877	Crystal structures of 4-bromo-2-formyl-1-tosyl-1H-pyrrole, $(E)-4-bromo-2-(2-nitrovinyl)-1-tosyl-1H-pyrrole$ and 6-(4-bromo-1-tosylpyrrol-2-yl)-4,4-dimethyl-5-nitrohexan-2-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 341-345.	0.2	3
2878	Crystal structure of strontium hydrogen citrate monohydrate, $Sr(HC_6H_5O_7)(H_2O)$ . <i>Powder Diffraction</i> , 2021, 36, 120-128.	0.4	1
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2882	Oxidative Addition of Hydridic, Protic, and Nonpolar E-H Bonds (E = Si, P, N, or O) to an Aluminylium Anion. <i>Inorganic Chemistry</i> , 2021, 60, 4772-4778.	1.9	21

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2885	Structural and theoretical studies of 4-chloro-2-methyl-6-oxo-3,6-dideuteropyrimidin-1-ium chloride ( $\text{C}_{10}\text{H}_{10}\text{ClN}_2\text{O}_2$ ). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 390-395.	0.2	1
2886	Crystal structure and Hirshfeld surface analysis of a copper(II) complex containing 2-nitrobenzoate and tetramethylethylenediamine ligands. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 412-415.	0.2	1
2887	Maleate salts of bedaquiline. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 433-445.	0.2	2
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2890	Crystal structure, Hirshfeld surface analysis and density functional theory study of 6-methyl-2-[(5-methylisoxazol-3-yl)methyl]-1H-benzimidazole. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 396-401.	0.2	3
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2892	Structural and Spectroscopic Comparison of Soft Se vs. Hard O Donor Bonding in Trivalent Americium/Neodymium Molecules. <i>Angewandte Chemie</i> , 2021, 133, 9545-9552.	1.6	4
2893	Supramolecular Self-Assembly Built by Weak Hydrogen, Chalcogen, and Unorthodox Nonbonded Motifs in 4-(4-Chlorophenyl)-3-[(4-fluorobenzyl)sulfanyl]-5-(thiophen-2-yl)-4H-1,2,4-triazole, a Selective COX-2 Inhibitor: Insights from X-ray and Theoretical Studies. <i>ACS Omega</i> , 2021, 6, 6996-7007.	1.6	5
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2896	Synthesis and Properties of Hybrid Halobismuthates of N-Acetylpyridinium Derivatives. <i>Russian Journal of Inorganic Chemistry</i> , 2021, 66, 482-489.	0.3	7
2897	Different patterns of supramolecular aggregation in three amides containing N-(benzo[thiazolyl]) substituents. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 504-511.	0.2	0
2898	Crystal structure and Hirshfeld surface analysis of 4,5-dibromo-2-(4-methoxyphenyl)-2,3,4,4a,5,6,7,7a-octahydro-1H-4,6-epoxy-1H-cyclopenta[ <i>c</i> ]pyridin-1-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 532-536.		
2899	Polymorphism and Supramolecular Isomerism: The Impasse of Coordination Polymers. , 0, , .		2
2900	Transition-metal complexes of group 12 with 1,1'-bis(phosphanyl)ferrocene ligands. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 240-248.	0.2	2

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2902	Predicting Energetics Materials' Crystalline Density from Chemical Structure by Machine Learning. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2147-2158.	2.5	28
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3023	Varying degrees of homostructurality in a series of cocrystals of antimalarial drug 11-azaartemisinin with salicylic acids. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 262-270.	0.2	4
3024	Synthesis, Spectral Characterization and Crystal Structures of Five Organic Ammonium Tetrasulfidomolybdates. <i>ChemistrySelect</i> , 2021, 6, 4750-4760.	0.7	0
3025	1/4-Methylene-bis[dibromido(diethyl ether- $\lambda^5$ -O)]aluminium(III): crystal structure and chemical exchange in solution. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 647-652.	0.2	0
3026	Crystal structure of diaqua(3,14-diethyl-2,6,13,17-tetraazatricyclo[16.4.0.0 <sup>7,12</sup> ] <sup>7,12</sup> ]docosane)copper(II) (3,14-diethyl-2,6,13,17-tetraazatricyclo[16.4.0.0 <sup>7,12</sup> ] <sup>7,12</sup> ]docosane)copper(II) tetrabromide dihydrate, [Cu(C <sub>22</sub> H <sub>44</sub> N <sub>4</sub> )(H <sub>2</sub> O) <sub>2</sub> ][Cu(C <sub>22</sub> H <sub>44</sub> N <sub>4</sub> ) <sub>2</sub> Br <sub>4</sub> ]	0.2	0
3027	Crystal structure and Hirshfeld surface analysis of bis(6,7,8,9-tetrahydro-1 <i>H</i> -pyrido[2,1- <i>b</i> ]quinazolin-5-ium) tetrachloridozincate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 629-633.	0.2	1
3028	Structural effects of meso-halogenation on porphyrins. <i>Beilstein Journal of Organic Chemistry</i> , 2021, 17, 1149-1170.	1.3	2
3029	Development of a Nanocrystal Formulation of a Low Melting Point API Following a Quality by Design Approach. <i>Processes</i> , 2021, 9, 954.	1.3	7

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3031	Elucidating the Origins of a Range of Diverse Flexible Responses in Crystalline Coordination Polymers. <i>Chemistry of Materials</i> , 2021, 33, 3660-3668.	3.2	22
3032	Crystal Engineering Using Polyiodide Halogen and Chalcogen Bonding to Isolate the Phenothiazinium Radical Cation and Its Rare Dimer, 10- $\pi$ -Phenothiazinylidene)phenothiazinium. <i>Chemistry - A European Journal</i> , 2021, 27, 8398-8405.	1.7	8
3033	Exploring Avenues beyond Revised DSD Functionals: I. Range Separation, with <i>x</i> -DSD as a Special Case. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4614-4627.	1.1	29
3034	Multicomponent Crystals of Chlorpropamide: Multiple Conformers, Multiple <i>Z</i> <sup>2</sup> , and Proton Transfer at Play. <i>Crystal Growth and Design</i> , 2021, 21, 3158-3167.	1.4	2
3035	Spodium bonding and other non-covalent interactions assisted supramolecular aggregation in a new mercury(II) complex of a nicotinohydrazide derivative. <i>Inorganica Chimica Acta</i> , 2021, 519, 120279.	1.2	25
3036	Crystal structure and molecular docking study of ( <i>E</i> )-2-[( <i>E</i> )-2-hydroxy-5-methylbenzylidene]hydrazinylidene}-1,2-diphenylethan-1-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 658-662.	0.2	3
3037	Visual pH Sensors: From a Chemical Perspective to New Bioengineered Materials. <i>Molecules</i> , 2021, 26, 2952.	1.7	34
3038	Investigations toward a Non-Aqueous Hybrid Redox-Flow Battery with a Manganese-Based Anolyte and Catholyte. <i>Advanced Energy Materials</i> , 2021, 11, 2101261.	10.2	4
3039	Structural insight from intermolecular interactions and energy framework analyses of 2-substituted 6,7,8,9-tetrahydro-11 <i>H</i> -pyrido[2,1- <i>b</i> ]quinazolin-11-ones. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 416-426.	0.5	2
3040	Molecular, Solid-State and Surface Structures of the Conformational Polymorphic Forms of Ritonavir in Relation to their Physicochemical Properties. <i>Pharmaceutical Research</i> , 2021, 38, 971-990.	1.7	24
3041	Phase solubility investigation and theoretical calculations on drug-drug cocrystals of carbamazepine with Emodin, Paeonol. <i>Journal of Molecular Liquids</i> , 2021, 329, 115604.	2.3	21
3042	Computational Identification of Novel Families of Nonfullerene Acceptors by Modification of Known Compounds. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5009-5015.	2.1	19
3043	Predicting inorganic dimensionality in templated metal oxides. <i>Journal of Chemical Physics</i> , 2021, 154, 184708.	1.2	6
3044	Contributions of secondary alcohol-ketone $\text{H}\cdots\text{O}=\text{C}$ and furan-acetate $\text{C}=\text{O}\cdots\text{H}\cdots\text{O}=\text{C}$ synthons to the supramolecular packings of two bioactive molecules. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 312-320.	0.2	0
3045	Bis(2-nitrophenyl) selenide, bis(2-aminophenyl) selenide and bis(2-aminophenyl) telluride: structural and theoretical analysis. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 271-280.	0.2	3
3046	Crystal structure and photoreactive behaviour of <i>N,N</i> -diisopropyl( <i>p</i> -phenylphenyl)glyoxylamide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 653-657.	0.2	1
3047	Crystal structure and Hirshfeld surface analysis of 2-(2-oxo-3-phenyl-1,2,3,8a-tetrahydroquinoxalin-1-yl)ethyl acetate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 643-646.	0.2	0



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3048	Assessing the potential of para-donor and para-acceptor substituted 5-benzylidenebarbituric acid derivatives as push-pull electronic systems: Experimental and quantum chemical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 253, 119576.	2.0	1
3049	Hydrogen-bond directionality and symmetry in [C(O)NH](N) <sub>2</sub> P(O)-based structures: a comparison between X-ray crystallography data and neutron-normalized values, and evaluation of reliability. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 384-396.	0.5	4
3050	A Combined Experimental and Computational Study of Halogen and Hydrogen Bonding in Molecular Salts of 5-Bromocytosine. <i>Molecules</i> , 2021, 26, 3111.	1.7	1
3051	Revisiting stacking interactions in tetrathiafulvalene and selected derivatives using tight-binding quantum chemical calculations and local coupled-cluster method. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 311-320.	0.5	6
3052	Stepwise Introduction of Flexibility into Aromatic Dicarboxylates Forming Uranyl Ion Coordination Polymers: a Comparison of 2-Carboxyphenylacetate and 1,2-Phenylenediacetate. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 2182-2192.	1.0	6
3053	Triazole-Based Half-Sandwich Ruthenium(II) Compounds: From <i>In Vitro</i> Antiproliferative Potential to <i>In Vivo</i> Toxicity Evaluation. <i>Inorganic Chemistry</i> , 2021, 60, 8011-8026.	1.9	7
3054	Analysis of Intermolecular Weak Interactions and Vibrational Characteristics for Vanillin and Ortho-Vanillin by Terahertz Spectroscopy and Density Functional Theory. <i>IEEE Transactions on Terahertz Science and Technology</i> , 2021, 11, 318-329.	2.0	15
3055	The Amine Group as Halogen Bond Acceptor in Cocrystals of Aromatic Diamines and Perfluorinated Iodobenzenes. <i>Crystals</i> , 2021, 11, 529.	1.0	13
3056	The First Insight Into the Supramolecular System of D,L-±-Difluoromethylornithine: A New Antiviral Perspective. <i>Frontiers in Chemistry</i> , 2021, 9, 679776.	1.8	7
3057	Comments on the paper "Growth and investigation of novel nonlinear optical single crystal of urea potassium dichromate by solution growth technique for photonic application". <i>Journal of Optics (India)</i> , 2022, 51, 767-771.	0.8	2
3058	Bis(2-methylpyridinium) tetrachloridocuprate(II): synthesis, structure and Hirshfeld surface analysis. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 726-729.	0.2	3
3059	Crystal structures of 9-[bis(benzylsulfanyl)methyl]anthracene and of cyclo-dodecakis(¼-phenylmethanethiolato) <sup>2-</sup> Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 302 Pd <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 718-725.	0.2	0
3060	Crystal structure, Hirshfeld and electronic transition analysis of 2-[(1 <i>H</i> -benzimidazol-1-yl)methyl]benzoic acid. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 755-758.	0.2	2
3061	Synthesis and crystal structure of a one-dimensional chain-like strontium(II) coordination polymer built of <i>N</i> -methyl-diethanolamine and isobutyrate ligands. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 703-707.	0.2	0
3062	A 3D MOF based on Adamantoid Tetracopper(II) and Aminophosphine Oxide Cages: Structural Features and Magnetic and Catalytic Properties. <i>Inorganic Chemistry</i> , 2021, 60, 9631-9644.	1.9	7
3063	Structural Landscape of Zn(II) and Cd(II) Coordination Compounds with Two Isomeric Triimidazole Luminophores: Impact of Crystal Packing Patterns on Emission Properties. <i>Crystal Growth and Design</i> , 2021, 21, 4184-4200.	1.4	8
3064	Structural and vibrational characterization of 1-(diaminomethylene)-thiourea-1-ium 4-aminobenzoate. <i>Journal of Molecular Structure</i> , 2021, 1234, 130181.	1.8	1
3065	A New Parameterization of an All-Atom Force Field for Cellulose. <i>Jom</i> , 2021, 73, 2335-2346.	0.9	0



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3067	Structural investigations into a new polymorph of F <sub>4</sub> TCNQ: towards enhanced semiconductor properties. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 426-434.	0.2	2
3068	One- and two-dimensional Pb <sup>II</sup> compounds resulting from reaction of PbBr <sub>2</sub> and Pb(SCN) <sub>2</sub> with pyrimidine-2-thione. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 402-410.	0.2	1
3069	Crystal structure of palbociclib isethionate Form B, (C <sub>24</sub> H <sub>30</sub> N <sub>7</sub> O <sub>2</sub> )(C <sub>2</sub> H <sub>5</sub> O <sub>4</sub> ·S). <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 196-201.	0.2	0
3070	Synthesis, structural characterization and antimycobacterial evaluation of several halogenated non-nitro benzothiazinones. <i>Medicinal Chemistry Research</i> , 2021, 30, 1523-1533.	1.1	9
3071	Crystal structure and Hirshfeld surface analysis of dimethyl 5-[2-(2,4,6-trioxo-1,3-diazinan-5-ylidene)hydrazin-1-yl]benzene-1,3-dicarboxylate 0.224-hydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 759-764.	0.2	0
3072	Crystal structure and magnetic study of the complex salt [RuCp(PTA) <sub>2</sub> ·½CN-1]·[RuCp(PTA) <sub>2</sub> ][Re(NO)Br <sub>4</sub> (EtOH) <sub>0.5</sub> ]. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 749-754.	0.2	0
3073	Hexanuclear copper(II) complex of 2-hydroxy- <i>N,N'</i> -bis[1-(2-hydroxyphenyl)ethylidene]propane-1,3-diamine incorporating an open-cubane core. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 708-713.	0.2	5
3074	<sup>31</sup> P NMR Chemical Shift Tensors: Windows into Ruthenium Phosphinidene Complex Electronic Structures. <i>Inorganic Chemistry</i> , 2021, 60, 9254-9258.	1.9	8
3075	Investigating the Role of Weak Interactions to Explore the Polymorphic Diversity in Difluorinated Isomeric <i>N</i> -Phenylcinnamamides. <i>Crystal Growth and Design</i> , 2021, 21, 4162-4177.	1.4	7
3076	Supramolecular interactions in the heteroarylimine-substituted calix[4]arenes: the formation of cyclic dodecanuclear palladium aggregates. <i>Supramolecular Chemistry</i> , 0, , 1-14.	1.5	0
3077	Powder X-ray diffraction of varenicline hydrogen tartrate Form B (Chantix <sup>®</sup> ), (C <sub>13</sub> H <sub>14</sub> N <sub>3</sub> )(HC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> ). <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 202-204.	0.4	0
3078	Synthesis and structures of a family of hybrid donor N <sub>2</sub> P <sub>2</sub> beta-diketiminato zinc complexes. <i>Polyhedron</i> , 2021, 201, 115150.	1.0	5
3079	Time-Dependent Self-Assembly of Copper(II) Coordination Polymers and Tetranuclear Rings: Catalysts for Oxidative Functionalization of Saturated Hydrocarbons. <i>Inorganic Chemistry</i> , 2021, 60, 14491-14503.	1.9	4
3080	A data-oriented approach to making new molecules as a student experiment: artificial intelligence-enabling FAIR publication of NMR data for organic esters. <i>Magnetic Resonance in Chemistry</i> , 2022, 60, 93-103.	1.1	9
3081	Synthesis, crystal structure determination, and spectroscopic analyses of 1-chloro-2-(2,6-diisopropylphenyl)-4,4-dimethyl-2-azaspiro[5.5]undecane-3,5-dione: an unyielding precursor to a cyclic (alkyl)(amido)carbene. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 411-419.	0.2	0
3082	Microsolvation of the Be-F bond in complexes of BeF <sub>2</sub> , BeF <sub>3</sub> <sup>-1</sup> , and BeF <sub>4</sub> <sup>-2</sup> with nH <sub>2</sub> O, for n=6, 8. <i>Molecular Physics</i> , 0, , e1933637.	0.8	2
3083	Copper(II) 2,2-Bis(Hydroxymethyl)Propionate Coordination Compounds with Hexamethylenetetramine: From Mononuclear Complex to One-Dimensional Coordination Polymer. <i>Molecules</i> , 2021, 26, 3358.	1.7	1
3084	Structural, physicochemical and biological characterization of chloramphenicol multicomponent complexes. <i>Journal of Molecular Liquids</i> , 2021, 331, 115761.	2.3	9

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3085	Growth, morphology and molecular orientation of controlled Indigo thin films on silica surfaces. <i>Surfaces and Interfaces</i> , 2021, 24, 101058.	1.5	6
3086	Highs and Lows of Bond Lengths: Is There Any Limit?. <i>Angewandte Chemie</i> , 2021, 133, 17165-17173.	1.6	5
3087	<i>cis</i> -Bis( <i>L</i> -DOPA) <sup>2+</sup> <i>N</i> , <i>O</i> -copper(II) monohydrate: synthesis, crystal structure, and approaches to the analysis of pseudosymmetry. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 383-390.	0.2	2
3088	Broken symmetry between RNA enantiomers in a crystal lattice. <i>Nucleic Acids Research</i> , 2021, 49, 12535-12539.	6.5	1
3089	On the nature of inter- and intramolecular interactions involving benzo[h]quinoline and 10-hydroxybenzo[h]quinoline: Electronic ground state vs excited state study. <i>Journal of Molecular Structure</i> , 2021, 1234, 130126.	1.8	7
3090	Structural Evolution in the RE(OAc) <sub>3</sub> · 2AcOH Structure Type. A Non-Linear, One-Dimensional Coordination Polymer with Unequal Interatomic Rare Earth Distances. <i>Crystals</i> , 2021, 11, 768.	1.0	1
3091	Crystal structure analysis and supramolecular association in ethyl <i>N</i> -[amino(iminio)methyl]carbamate dichloride hemi-hydrate. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2021, 236, 187-199.	0.4	0
3092	Mechanochemistry as a Reconstruction Tool of Decomposed Metal-Organic Frameworks. <i>Inorganic Chemistry</i> , 2021, 60, 11825-11829.	1.9	11
3093	<i>cyclo</i> -Tetrakis(1/4-2,4,6-trimethylphenyl) <i>C</i> <sup>1</sup> Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 422 1 Td ( <sup>1</sup> )	0.1	1
3094	Synthesis and characterization of the Anderson-Evans tungstoantimonate [Na <sub>5</sub> (H <sub>2</sub> O) <sub>18</sub> {(HOCH <sub>2</sub> ) <sub>2</sub> CHNH <sub>3</sub> } <sub>2</sub> ][SbW <sub>12</sub> O <sub>42</sub> ]. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 420-425.	0.2	1
3095	Tautomeric Equilibrium of an Asymmetric 1,2-Diketone in Halogen-Bonded Cocrystals with Perfluorinated Iodobenzenes. <i>Crystals</i> , 2021, 11, 699.	1.0	7
3096	ANION-CATION VERSUS WEAK INTERMOLECULAR INTERACTIONS IN THE STRUCTURES OF Et <sub>4</sub> N <sup>+</sup> , Pr <sub>4</sub> N <sup>+</sup> , AND Bu <sub>4</sub> N <sup>+</sup> CATION SALTS WITH THE [W(CN) <sub>6</sub> (bpy)] <sup>2-</sup> ANION. <i>Journal of Structural Chemistry</i> , 2021, 62, 905-917.	0.3	6
3097	Advances in adsorptive separation of benzene and cyclohexane by metal-organic framework adsorbents. <i>Coordination Chemistry Reviews</i> , 2021, 437, 213852.	9.5	74
3098	Controlled Light and Temperature Induced Valence Tautomerism in a Cobalt-o-Dioxolene Complex. <i>Inorganic Chemistry</i> , 2021, 60, 8665-8671.	1.9	5
3099	Refinement of K[Hg <sub>3</sub> ]H <sub>2</sub> O using non-spherical atomic form factors. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 681-685.	0.2	1
3100	Signature of Glycylglutamic Acid Structure. <i>International Journal of Biochemistry and Biophysics</i> , 2021, 9, 8-15.	0.5	1
3101	Alkali metal salts of 4-hydroxybenzoic acid: a structural and educational study. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 340-353.	0.2	3
3102	Zinc(II) and nickel(II) complexes of 3,5-dimethyl-1-(pyridin-2-yl)-1 <i>H</i> -pyrazole: relationship between fluorescence and crystal packing. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 321-330.	0.2	1

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3103	Crystal structure and optical properties of a two-sided Eu <sup>III</sup> compound: an Eu <sup>III</sup> ion coordinated by two [Eu <sup>III</sup> (DOTA)] <sup>-</sup> complexes (DOTA is Tj ETQq0 0,2 rgBT /Qverlock 10 Chemistry, 2021, 77, 354-364.	0.2	0
3104	Solvent-Dependent Impact of Spectator Anions on the Thermodynamics of Cation Exchange in CdSe Nanocrystals. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12792-12801.	1.5	5
3105	Highs and Lows of Bond Lengths: Is There Any Limit?. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 17028-17036.	7.2	13
3106	Boron-Doped MXenes as Electrocatalysts for Nitrogen Reduction Reaction: A Theoretical Study. <i>Frontiers in Chemical Engineering</i> , 2021, 3, .	1.3	4
3107	Tetraammonium bis(metforminium) di- $\frac{1}{4}$ -oxido-tetra- $\frac{1}{4}$ -oxido-tetradeca- $\frac{1}{4}$ -oxido-2-oxido-octaoxidodecavanadium(V) hexahydrate. <i>IUCrData</i> , 2021, 6, .	0.1	2
3108	Chalcogen S <sup>TM</sup> â <sup>TM</sup> â <sup>TM</sup> MS Bonding in Supramolecular Assemblies of Cadmium(II) Coordination Polymers with Pyridine-Based Ligands. <i>Crystals</i> , 2021, 11, 697.	1.0	1
3109	Isorecticular Chemistry of Group 13 Metalâ€“Organic Framework Compounds Based on V-Shaped Linker Molecules: Exceptions to the Rule?. <i>Inorganic Chemistry</i> , 2021, 60, 8861-8869.	1.9	4
3110	The Detosylation of Chiral 1,2-Bis(tosylamides). <i>Journal of Organic Chemistry</i> , 2021, 86, 9163-9180.	1.7	5
3112	Synthesis, structural and in vitro biological evaluation of diamondoid-decorated lipophilic organotin(IV) derivatives. <i>Journal of Organometallic Chemistry</i> , 2021, 941, 121802.	0.8	6
3113	Insights on a new sulfonamide chalcone with potential antineoplastic application. <i>Journal of Molecular Modeling</i> , 2021, 27, 211.	0.8	3
3114	Two Cu(II) complexes involving halogen bonding interactions. <i>Molecular Crystals and Liquid Crystals</i> , 2021, 722, 58-66.	0.4	0
3115	Promotion and Tuning of the Electrochemical Reduction of Heteroâ€“and Homobimetallic Zinc Complexes**. <i>ChemElectroChem</i> , 2021, 8, 2792-2802.	1.7	5
3116	Crystal structure and Hirshfeld surface analysis of ethyl 6â€“amino-2â€“(chloromethyl)-5â€“cyano-2-oxo-1,2-dihydrospiro[indoline-3,4â€“pyran]-3â€“carboxylate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 739-743.	0.2	1
3117	Crystal structure of 1,2-bis(3,5-difluorophenyl)ethane-1,2-dione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 700-702.	0.2	0
3118	Synthesis and crystal structure of poly[(3-amino-1,2,4-triazole)( $\frac{1}{4}$ -1 <i>H</i> -benzimidazole-5,6-dicarboxylato)cobalt(II)]. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 714-717.	0.2	0
3119	Rapid SERS Quantification of Trace Fentanyl Laced in Recreational Drugs with a Portable Raman Module. <i>Analytical Chemistry</i> , 2021, 93, 9373-9382.	3.2	34
3120	Crystal Structure Prediction Methods for Organic Molecules: State of the Art. <i>Annual Review of Chemical and Biomolecular Engineering</i> , 2021, 12, 593-623.	3.3	28
3121	The Good, the Bad, and the Twisted Revisited: An Analysis of Ligand Geometry in Highly Resolved Proteinâ€“Ligand X-ray Structures. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 7533-7543.	2.9	13

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3122	Keine Kosten, viel Spaß. Nachrichten Aus Der Chemie, 2021, 69, 10-12.	0.0	0
3123	Efficient Molybdenum Hydrazonato Epoxidation Catalysts Operating under Green Chemistry Conditions: Water vs. Decane Competition. <i>Catalysts</i> , 2021, 11, 756.	1.6	3
3124	Crystal structure and Hirshfeld surface analysis of ethyl 2-({5-acetyl-3-cyano-6-methyl-4-[( <i>E</i> )-2-phenylethenyl]pyridin-2-yl}sulfanyl)acetate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 730-733.	0.2	0
3125	Non-Covalent Interactions in the Biphenyl Crystal: Is the Planar Conformer a Transition State?. <i>Chemistry - A European Journal</i> , 2021, 27, 11912-11918.	1.7	14
3126	Pyridinium 3-nitrobenzoate-3-nitrobenzoic acid (1/1). <i>IUCrData</i> , 2021, 6, .	0.1	0
3127	Theoretical and Experimental Insights into the Tandem Mannich Electrophilic Amination Reaction: Synthesis of Safirinium Dyes. <i>Applied Sciences (Switzerland)</i> , 2021, 11, 5498.	1.3	1
3128	The Quest for Optimal $d$ Orbital Splitting in Tetrahedral Cobalt Single-Molecule Magnets Featuring Colossal Anisotropy and Hysteresis. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 3108-3114.	1.0	13
3129	$\beta$ -Cyclodextrin Inclusion Complexes with Catechol-Containing Antioxidants Protocatechuic Aldehyde and Protocatechuic Acid: An Atomistic Perspective on Structural and Thermodynamic Stabilities. <i>Molecules</i> , 2021, 26, 3574.	1.7	9
3130	Molecular structures of the pentaphenylcyclopentadienyl iron complexes [(C <sub>5</sub> Ph <sub>5</sub> )Fe(CO) <sub>2</sub> R] (R = Me, Ph, <i>i</i> Pr and Bu). <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 374-382.	0.2	1
3131	Lanthanide Coordination Polymers through Design for Exceptional Catalytic Performances in CO <sub>2</sub> Cycloaddition Reactions. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 8581-8591.	3.2	23
3132	Structural and Thermal Investigations of Co(II) and Ni(II) Coordination Polymers Based on biphenyl-4,4'-dioxidiacetate Linker. <i>Materials</i> , 2021, 14, 3545.	1.3	3
3133	Inclusion of citral isomers in native and methylated cyclodextrins: Structural insights by X-ray crystallography and molecular dynamics simulation analysis. <i>Journal of Molecular Structure</i> , 2021, 1234, 130169.	1.8	5
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3175	Crystal structure and Hirshfeld surface analysis of (3 <i>R</i> ,4 <i>S</i> ,7 <i>S</i> ,7 <i>a</i> <i>S</i> )-4,5,6,7,8-hexachloro-2-[6-[(3 <i>R</i> ,4 <i>R</i> ,7 <i>R</i> ,7 <i>a</i> <i>S</i> )-4,5,6,7,8-hexachloro-2-oxo-2-phenylethyl]pyridin-2-yl]pyridine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 775-779.		



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3341	Crystal structure of 2-{[5-amino-1-(phenylsulfonyl)-1H-pyrazol-3-yl]oxy}-1-(4-methylphenyl)ethan-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2021, 77, 1054-1057.	0.2	3
3342	Crystal and molecular structures of some phosphane-substituted cymantrenes [(C <sub>5</sub> H <sub>4</sub> X)Mn(CO) <sub>2</sub> ] (X = H or Cl, L = CO, L = Tj ETQq 1 0.784)	0.2	0
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3377	Exploring packing features of N-substituted acridone derivatives: Synthesis and X-ray crystallography studies. <i>Journal of Molecular Structure</i> , 2022, 1248, 131448.	1.8	3
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3380	Synthesis and structure of (E)-N-(4-methoxyphenyl)-2-[4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy]acetamide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 184-189.	0.2	1
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3525	Influence of the position of the methyl substituent and N-oxide formation on the geometry and intermolecular interactions of 1-(phenoxyethyl)piperidin-4-ol derivatives. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 30-36.	0.2	5
3526	Biological properties of two enantiomeric forms of N-(2,6-dimethylphenyl)-4-hydroxy-2,2-dioxo-1H-pyridin-2-ylidene-1-benzothiazine-3-carboxamide, a structural analogue of piroxicam. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 69-74.	0.2	3
3527	Conformational flexibility in amidophosphoesters: a CSD analysis completed with two new crystal structures of (C <sub>6</sub> H <sub>5</sub> O) <sub>2</sub> P(O)X [X = NHC <sub>7</sub> H <sub>13</sub> and N(CH <sub>2</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ]. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 104-116.	0.2	6
3528	Bond length of perchlorate at different temperatures: X-ray and neutron comparison. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 159-163.	0.2	1
3529	Solvent influence on the crystal packing of 6-aminothiocytosine. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 250-257.	0.2	3
3530	Playing around with MP, a tool for the analysis of pseudosymmetry: recurrent appearance of local pseudo-space groups in the asymmetric unit of Z = 4 structures. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 258-268.	0.2	6
3531	Bases, solvates and salts: new benzimidazole- and pyridine-scaffolded ligands. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 367-374.	0.2	2
3532	Synthesis of N-substituted 3-(2-aryl-2-oxoethyl)-3-hydroxyindolin-2-ones and their conversion to N-substituted (E)-3-(2-aryl-2-oxoethylidene)indolin-2-ones: synthetic sequence, spectroscopic characterization and structures of four 3-hydroxy compounds and five oxoethylidene products. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 433-445.	0.2	2
3533	Synthesis, decomposition studies and crystal structure of a three-dimensional CuCN network structure with protonated N-methylethanolamine as the guest cation. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 405-411.	0.2	1
3534	A 2D coordination polymer assembled from a nickel(II) tetraazamacrocyclic cation and 4,4'-bis(dimethylsilanediyloxy)diphthalate(3-) linker. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 419-426.	0.2	4
3535	Crystal structures, packing features, Hirshfeld surface analyses and DFT calculations of hydrogen-bond energy of two homologous 8a-aryl-2,3,4,7,8,8a-hexahydropyrrolo[1,2-a]pyrimidin-6(1H)-ones. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 483-489.	0.2	2
3536	Can we trust the experiment? Anisotropic displacement parameters in 1-(halomethyl)-3-nitrobenzene (halogen = Cl or Br). <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 591-597.	0.2	2
3537	Intermolecular interactions and disorder in six isostructural celecoxib solvates. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 632-638.	0.2	6
3538	Crystal structures of salts of bedaquiline. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 1010-1023.	0.2	7

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3539	Aspherical scattering factors for SHELXL model, implementation and application. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 50-62.	0.0	49
3540	Aspects of the topology of actinide atom substructures in crystal structures and the concept of antiliquid. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 370-378.	0.0	6
3541	Extension of the transferable aspherical pseudoatom data bank for the comparison of molecular electrostatic potentials in structure activity studies. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 398-408.	0.0	25
3542	Crystal structure of tris(trans-1,2-cyclohexanediamine- $\hat{N}$ 2N, $\hat{N}$ $\hat{C}$ 2)chromium(III) tetrachloridozincate chloride trihydrate from synchrotron data. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 671-674.	0.2	3
3543	Crystal structure and hydrogen bonding in the water-stabilized proton-transfer salt brucinium 4-aminophenylarsonate tetrahydrate. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 751-755.	0.2	3
3544	Crystal structure of phenyl 2,4,5-trichlorobenzenesulfonate. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 789-792.	0.2	3
3545	Crystal structure of [tris(pyridin-2-ylmethyl)amine- $\hat{N}$ 4N]copper(II) bromide. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 801-804.	0.2	3
3546	Crystal structure of 1,3-bis(1 <i>H</i> -benzotriazol-1-ylmethyl)benzene. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 815-818.	0.2	3
3547	A kryptoracemic salt: 2-[[2,8-bis(trifluoromethyl)quinolin-4-yl](hydroxy)methyl]piperidin-1-ium (+)-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 872-877.	0.2	4
3548	Crystal structures of three 6-substituted coumarin-3-carboxamide derivatives. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 926-932.	0.2	14
3549	Crystal structure of bis{4-bromo-2-[(carbamidamidoimino)methyl]phenolato- $\hat{N}$ 3N, $\hat{N}$ $\hat{C}$ 2,O}cobalt(III) nitrate dimethylformamide monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 907-911.	0.2	3
3550	Crystal structure of bis(isonicotinamide- $\hat{N}$ 1)bis(thiocyanato- $\hat{N}$ 2N)zinc. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 922-925.	0.2	4
3551	Crystal structure of diaquabis(7-diethylamino-3-formyl-2-oxo-2 <i>H</i> -chromen-4-olato- $\hat{N}$ 2 <sup>2</sup> <i>O</i> <sup>3</sup> , <i>O</i> <sup>4</sup> <sub>2</sub> )zinc dimethyl sulfoxide disolvate. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1032-1036.	0.2	2
3552	$\hat{N}$ $\hat{C}$ 2-[(1E)-(5-Nitrofur-2-yl)methylidene]thiophene-2-carbohydrazide: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1025-1031.	0.2	4
3553	Crystal structure of 4-methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1021-1024.	0.2	1
3554	$\hat{N}$ $\hat{C}$ 2-[(1E)-(5-Nitrofur-2-yl)methylidene]thiophene-2-carbohydrazide: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1085-1092.	0.2	10
3555	Crystal structure of glycidamide: the mutagenic and genotoxic metabolite of acrylamide. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1179-1182.	0.2	4
3556	6-Methyl-2-oxo- <i>N</i> -(quinolin-6-yl)-2 <i>H</i> -chromene-3-carboxamide: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1121-1125.	0.2	2

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3557	Crystal structure of 2-methyl-1 <i>H</i> -imidazol-3-ium hydrogen oxalate dihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1113-1115.	0.2	5
3558	Crystal structure of bergapten: a photomutagenic and photobiologically active furanocoumarin. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1194-1196.	0.2	8
3559	Distinct coordination geometries in bis[N,N-bis(2-methoxyethyl)dithiocarbamato- $\lambda^2$ S, $\lambda^2$ ]diphenyltin(IV) and bis[N-(2-methoxyethyl)-N-methyldithiocarbamato- $\lambda^2$ S, $\lambda^2$ ]diphenyltin(IV): crystal structures and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1130-1137.	0.2	6
3560	Crystal structure of ammonium/potassiumtrans-bis(N-methyliminodiacetato- $\lambda^3$ O,N, $\lambda^2$ )chromate(III) from synchrotron data. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1190-1193.	0.2	3
3561	Isotypic one-dimensional coordination polymers:catena-poly[[dichloridocadmium]- $\lambda^1$ 4-5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylato- $\lambda^2$ N5:N6] andcatena-poly[[dichloridomercury(II)]- $\lambda^1$ 4-5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylato- $\lambda^2$ N5:N6]. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1214-1218.	0.2	2
3562	An unprecedented binuclear cadmium dithiocarbamate adduct: bis[ $\lambda^1$ 4- $\lambda^2$ 2-(2-hydroxyethyl)- $\lambda^1$ 2-isopropylcarbamodithioato- $\lambda^3$ S, $\lambda^2$ ]bis(dihydrate). Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1234-1238.	0.2	1
3563	Crystal structure of methyl 3- $\lambda^2$ -benzamido-4- $\lambda^2$ -(4-methoxyphenyl)-1- $\lambda^2$ -methylspiro[indeno[1,2- <i>b</i> ]quinoxaline-11,2- $\lambda^2$ -pyrrolidine]-3- $\lambda^2$ -carboxylate. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1257-1259.	0.2	1
3564	Two forms of (naphthalen-1-yl)boronic acid. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1285-1289.	0.2	3
3565	Synthesis and crystal structure of tricarbonylchlorido{1-[(pyridin-2-ylmethylidene)amino]adamantane}rhenium(I). Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1276-1279.	0.2	1
3566	(+)- <i>trans</i> -Chlorido{2-[( <i>R</i> )-2-(methylsulfanyl)ferrocenyl]-2,5,6,7-tetrahydropyrrolo[1,2- <i>c</i> ]imidazol-3-yl}hexafluoridophosphate dichloroform disolvate. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1330-1334.	0.2	1
3567	Crystal structure of an aryl cyclohexyl nonanoid, an antiproliferative molecule isolated from the spice <i>Myristica malabarica</i> . Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1408-1411.	0.2	2
3568	Crystal structure of a second polymorph of tricarbonyl(N-methylpyridine-2-carboxamide- $\lambda^2$ N1,O)(thiocyanato- $\lambda^1$ N)rhenium(I). Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1386-1389.	0.2	1
3569	Crystal structure of 2-chloro-1,3-(2,6-diisopropylphenyl)-4,5-dihydro-1 <i>H</i> -imidazol-3-ium tetrakis(3,5-trifluoromethylphenyl)borate. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1471-1474.	0.2	1
3570	The crystal structure of 6-(4-chlorophenyl)-2-(4-methylbenzyl)imidazo[2,1- <i>b</i> ][1,3,4]thiadiazole-5-carbaldehyde. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1460-1462.	0.2	4
3571	[N-Benzyl-N-(2-phenylethyl)dithiocarbamato- $\lambda^2$ S, $\lambda^2$ ]triphenyltin(IV) and [bis(2-methoxyethyl)dithiocarbamato- $\lambda^2$ S, $\lambda^2$ ]triphenyltin(IV): crystal structures and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1480-1487.	0.2	4
3572	Halogen-bonded network of trinuclear copper(II) 4-iodopyrazolate complexes formed by mutual breakdown of chloroform and nanojars. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1517-1520.	0.2	7
3573	Crystal structure of di- $\lambda^1$ 4-chlorido-bis[chloridobis(1,2-dimethyl-5-nitro-1 <i>H</i> -imidazole- $\lambda^1$ N, $\lambda^3$ )copper(II)] acetonitrile disolvate. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1633-1636.	0.2	5
3574	Crystal structure of Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1595-1598.	0.2	1

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3575	Crystal and geometry-optimized structure, and Hirshfeld surface analysis of 1-(2-bromoethyl)indoline-2,3-dione. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1569-1573.	0.2	2
3576	Crystal structures of 3,3- $\epsilon^2$ -bis(hydroxydimethylsilyl)azobenzene and 4,4- $\epsilon^2$ -bis(hydroxydimethylsilyl)azobenzene. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1590-1594.	0.2	2
3577	Crystal structure of the 1:2 co-crystal of 1,3,6,8-tetraazatricyclo[4.3.1.1 <sup>3,8</sup> ]undecane (TATU) and 4-chlorophenol (1/2). Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1648-1650.	0.2	2
3578	Mechanochemical synthesis and crystal structure of a 1:2 co-crystal of 1,3,6,8-tetraazatricyclo[4.3.1.1 <sup>3,8</sup> ]undecane (TATU) and 4-chloro-3,5-dimethylphenol. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1651-1653.	0.2	2
3579	Channels with ordered water and bipyridine molecules in the porous coordination polymer $\{[\text{Cu}(\text{SiF}_6)(\text{C}_{10}\text{H}_8\text{N}_2)_2] \cdot 2\text{C}_{10}\text{H}_8\text{N}_2 \cdot 5\text{H}_2\text{O}\}_n$ . Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1654-1658.	0.2	1
3580	Crystal structure of aquatris[ $\frac{1}{4}$ -N-[bis(diethylamino)phosphoryl]-2,2,2-trichloroacetamido- $\hat{\nu}$ $^3\text{O}, \text{O}\hat{\nu}^2\text{:O}$ ]calciumsodium. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1683-1686.	0.2	4
3581	Crystal structures of four co-crystals of (E)-1,2-di(pyridin-4-yl)ethene with 4-alkoxybenzoic acids: 4-methoxybenzoic acid $\hat{\nu}$ “(E)-1,2-di(pyridin-4-yl)ethene (2/1), 4-ethoxybenzoic acid $\hat{\nu}$ “(E)-1,2-di(pyridin-4-yl)ethene (2/1), 4-n-propoxybenzoic acid $\hat{\nu}$ “(E)-1,2-di(pyridin-4-yl)ethene (2/1) and 4-n-butoxybenzoic acid $\hat{\nu}$ “(E)-1,2-di(pyridin-4-yl)ethene (2/1). Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1666-1671.	0.2	3
3582	Crystal structure of hexakis(dimethyl sulfoxide- $\hat{\nu}$ $\langle i \rangle \text{O} \langle /i \rangle$ )manganese(II) tetraiodide. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1791-1793.	0.2	5
3583	Crystal structure of bis(3,5-dimethylpyridine- $\hat{\nu}$ $\langle i \rangle \text{N}$ )bis(methanol- $\hat{\nu}$ $\langle i \rangle \text{O}$ )bis(thiocyanato- $\hat{\nu}$ $\langle i \rangle \text{N}$ )cobalt(II). Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1824-1826.	0.2	1
3584	Crystal structure of ( $\langle i \rangle \text{E} \langle /i \rangle$ )-9-([4-(diethylamino)phenyl]imino)methyl)-2,3,6,7-tetrahydro-1- $\langle i \rangle \text{H} \langle /i \rangle$ ,5- $\langle i \rangle \text{H} \langle /i \rangle$ -pyrido[3,2,1- $\langle i \rangle \text{ij} \langle /i \rangle$ ]quinolin-8-ol. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 38-40.		
3585	Crystal structure of 4-(4b,8a-dihydro-9- $\langle i \rangle \text{H} \langle /i \rangle$ -pyrido[3,4- $\langle i \rangle \text{bc} \langle /i \rangle$ ]indol-1-yl)-7-methyl-2- $\langle i \rangle \text{H} \langle /i \rangle$ -chromen-2-one. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 56-58.	0.2	1
3586	Crystal structure of bis[cis-(1,4,8,11-tetraazacyclotetradecane- $\hat{\nu}$ $\langle i \rangle 4\text{N}$ )bis(thiocyanato- $\hat{\nu}$ $\langle i \rangle \text{N}$ )chromium(III)] dichromate monohydrate from synchrotron X-ray diffraction data. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 72-75.	0.2	7
3587	Crystal structure of dirubidium hydrogen citrate from laboratory X-ray powder diffraction data and DFT comparison. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 92-95.	0.2	10
3588	Crystal structure of caesium dihydrogen citrate from laboratory X-ray powder diffraction data and DFT comparison. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 133-136.	0.2	5
3589	Crystal structures and hydrogen bonding in the isotopic series of hydrated alkali metal (K, Rb and Cs) complexes with 4-aminophenylarsonic acid. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 203-208.	0.2	6
3590	Crystal structure of trirubidium citrate monohydrate from laboratory X-ray powder diffraction data and DFT comparison. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 227-230.	0.2	9
3591	Crystal structure of chloridobis[(1,2,5,6- $\hat{\nu}$ )-cycloocta-1,5-diene]iridium(I). Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 273-277.	0.2	1
3592	Crystal structure of bis(1-ethylpyridinium) dioxonium hexacyanidoferrate(II). Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 219-222.	0.2	1



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3593	Crystal structure of trirubidium citrate from laboratory X-ray powder diffraction data and DFT comparison. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 250-253.	0.2	8
3594	Di- <i>n</i> -butylbis[ <i>N</i> -(2-methoxyethyl)- <i>N</i> -methylthiocarbamato- $\lambda^2$ - <i>S</i> , <i>S</i> ] $\lambda^2$ -tin(IV): crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 260-265.	0.2	10
3595	Four pyrrole derivatives used as building blocks in the synthesis of minor-groove binders. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 254-259.	0.2	2
3596	Crystal structure of $\lambda^4$ -chlorido-nonakis( $\lambda^4$ -4-chloropyrazolato)bis( $\lambda^4$ -3-methoxo-hexacopper(II)). Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 266-269.	0.2	5
3597	Bis{4-methylbenzyl 2-[4-(propan-2-yl)benzylidene]hydrazinecarbodithioato- $\lambda^2$ - <i>N</i> , <i>S</i> }nickel(II): crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 397-402.	0.2	3
3598	Crystal structures of three sterically congested disilanes. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 448-452.	0.2	1
3599	Bis( $\lambda^2$ - <i>N</i> -methyl- <i>N</i> -phenylthiocarbamato- $\lambda^2$ - <i>S</i> , <i>S</i> ; $\lambda^2$ - <i>S</i> , <i>S</i> -bis[( <i>N</i> -methyl- <i>N</i> -phenylthiocarbamato- $\lambda^2$ - <i>S</i> , <i>S</i> )cadmium]: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 429-433.	0.2	1
3600	Crystal structure of 6,7-dimethoxy-1-(4-nitrophenyl)quinolin-4(1 <i>H</i> )-one: a molecular scaffold for potential tubulin polymerization inhibitors. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 441-444.	0.2	1
3601	Crystal structures of <i>N</i> -(4-chlorophenyl)-2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]acetamide and <i>N</i> -(3-chlorophenyl)-2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]acetamide. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 467-471.	0.2	3
3602	Tricaesium citrate monohydrate, Cs <sub>3</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> ·H <sub>2</sub> O: crystal structure and DFT comparison. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 520-523.	0.2	3
3603	Crystal structure of bis(4-benzoylpyridine- $\lambda^2$ - <i>N</i> )bis(methanol- $\lambda^2$ - <i>O</i> )bis(thiocyanato- $\lambda^2$ - <i>N</i> )cobalt(II). Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 616-619.	0.2	4
3604	<i>trans</i> -Dichloridobis(dimethyl sulfoxide- $\lambda^2$ - <i>O</i> )bis(4-fluorobenzyl- $\lambda^2$ - <i>C</i> ) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 307 E: Crystallographic Communications, 2017, 73, 667-672.	0.2	9
3605	Crystal structure of the diglycidyl ether of eugenol. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 694-697.	0.2	4
3606	Crystal structure of ( <i>S</i> )- <i>sec</i> -butylammonium <i>L</i> -tartrate monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 716-719.	0.2	1
3607	Crystal structure of 1,4,8,11-tetraazoniacyclotetradecane bis(dichromate) monohydrate from synchrotron data. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 755-758.	0.2	3
3608	Crystal structure of di- $\lambda^4$ -chlorido-bis(chlorido{ <i>N</i> <sup>1</sup> , <i>N</i> <sup>1</sup> -diethyl- <i>N</i> <sup>4</sup> }-[(pyridin-2-yl- <i>N</i> )methy		
3609	Crystal structure of a new spiro-polytetrahydrofuran compound with translational pseudosymmetry: <i>rac</i> -(2 <i>S</i> ,2 <i>S</i> ,5 <i>R</i> )-2-methyl-5-[(1 <i>R</i> ,2 <i>R</i> ,5 <i>S</i> )-5- <i>R</i> ]-1,4,5-trimethyl-		
3610	An infinite two-dimensional hybrid water-chloride network in a $\lambda^2$ -(furan-2-yl)-2,2,6,2-terpyridine nickel(II) matrix. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 871-875.	0.2	1



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3611	Crystal structure of 4,4'-bis[3-(piperidin-1-yl)prop-1-yn-1-yl]-1,1'-biphenyl. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 864-866.	0.2	1
3612	2-[(4-Chlorophenyl)selenyl]-3,4-dihydro-2H-benzo[h]chromene-5,6-dione: crystal structure and Hirshfeld analysis. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 918-924.	0.2	3
3613	Crystal structure of N-(4-oxo-2-sulfanylidene-1,3-thiazolidin-3-yl)-2-(thiophen-3-yl)acetamide. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 901-904.	0.2	6
3614	C <sub>2</sub> -isomer of [Pd(tfd) <sub>6</sub> ][tfd] S <sub>2</sub> C <sub>2</sub> (CF <sub>3</sub> ) <sub>2</sub> as its benzene solvate: a new member of the small but growing class of homoleptic palladium(II) monodithiolenes in the form of hexameric cubes. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 957-962.	0.2	3
3615	Crystal structure of $\frac{1}{4}$ -oxalato- $\mu_2$ O1:O2-bis[(dimethyl sulfoxide- $\mu$ )triphenyltin(IV)]. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1033-1036.	0.2	1
3616	Crystal structure of N-[2-(benzo[d]thiazol-2-yl)acetyl]-4-methylbenzenesulfonohydrazide. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1041-1043.	0.2	16
3617	Crystal structure and UV spectra of a 1,2-disubstituted benzimidazolium chloride. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1143-1147.	0.2	3
3618	Ethyl 2-(4-methoxyphenyl)-6-oxa-3-azabicyclo[3.1.0]hexane-3-carboxylate: crystal structure and Hirshfeld analysis. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1218-1222.	0.2	7
3619	A new solvate of epalrestat, a drug for diabetic neuropathy. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1264-1267.	0.2	2
3620	Crystal structure of 1-[2-(4-nitrophenyl)-4,5-diphenyl-1H-imidazol-1-yl]propan-2-ol. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1398-1401.	0.2	1
3621	Bis( $\frac{1}{4}$ -N,N'-diallyldithiocarbamate)bis[(N,N'-diallyldithiocarbamate)cadmium]. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1353-1356.	0.2	2
3622	Bis(3,5-dimethoxy-2-[2-(pyridin-2-yl)ethylimino- $\mu$ N]methyl}phenolato- $\mu$ O)bis(dimethyl) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 3 Crystallographic Communications, 2017, 73, 1479-1482.	0.2	1
3623	Crystal structures of the dioxane hemisolates of N-(7-bromomethyl-1,8-naphthyridin-2-yl)acetamide and bis[N-(7-dibromomethyl-1,8-naphthyridin-2-yl)acetamide]. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1409-1413.	0.2	5
3624	A two-dimensional Zn coordination polymer with a three-dimensional supramolecular architecture. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1402-1404.	0.2	2
3625	Synthesis and crystal structures of two new tin bis(carboranylaminidate) complexes. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1443-1448.	0.2	2
3626	Crystal structure of flucetosulfuron. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1439-1442.	0.2	12
3627	Crystal structures of three hydrogen-bonded 1:2 compounds of chloranilic acid with 2-pyridone, 3-hydroxypyridine and 4-hydroxypyridine. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1546-1550.	0.2	3
3628	N,N',N''- versus N,N'-, N,N'-, N,O- imine-containing coordination motifs: ligand-directed synthesis of mononuclear and binuclear Cu <sup>II</sup> compounds. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1563-1567.	0.2	4

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3629	(E)-7-[(4-Nitrophenyl)diazanyl]-3a-(p-tolyl)-2,3,3a,4-tetrahydro-1H-benzo[d]pyrrolo[1,2-a]imidazol-1-one 0.58-dimethyl sulfoxide 0.42-acetonitrile solvate: crystal structure, Hirshfeld analysis and DFT estimation of the energy of intermolecular interactions. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1590-1594.	0.2	2
3630	1-[(E)-[(2E)-3-(4-Methoxyphenyl)-1-phenylprop-2-en-1-ylidene]amino]-3-phenylurea: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1607-1611.	0.2	2
3631	Crystal structure of methyl ( <i>Z</i> )-2-[( <i>Z</i> )-3-methyl-2-[( <i>E</i> )-1-[( <i>R</i> *)-4-methylcyclohex-3-en-1-yl]ethylidene]hydrazinylidene]-2-oxo-1,2,4-thiazolidin-5-one. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1626-1629.	0.2	2
3632	Stoichiometric and polymorphic salts of hexamethylenetetraminium and 2-chloro-4-nitrobenzoate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1630-1635.	0.2	1
3633	Crystal structures and Hirshfeld surfaces of differently substituted ( <i>E</i> )- <i>N</i> -benzylidene- <i>N</i> -methyl-2-(thiophen-2-yl)acetohydrazides. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1636-1641.	0.2	3
3634	Crystal structure of ( <i>Z</i> )- <i>N</i> -benzylidene-1-phenylmethanamine oxide hydrogen peroxide monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1666-1669.	0.2	5
3635	Green synthesis and crystal structure of 3-(benzothiazol-2-yl)thiophene. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1647-1651.	0.2	4
3636	Crystal structure of aqua(perchlorato)bis[1/4-( <i>E</i> )-2-[[2-(pyridin-2-yl)ethyl]imino]methyl]phenolato-1/4<sup>4</sup><math>\langle i \rangle N \langle i \rangle, \langle i \rangle N \langle i \rangle, \langle i \rangle O \langle i \rangle</math> perchlorate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1708-1711.	0.2	1
3637	A 2:1 co-crystal of 3,5-dibromo-4-cyanobenzoic acid and anthracene. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1743-1746.	0.2	4
3638	Crystal structure of bis(pyridine-4-carbothioamide-1 <i>N</i> )bis(thiocyanato-1 <i>N</i> )cobalt(II) methanol monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1786-1789.	0.2	2
3639	Crystal structure of tetraisobutylthiuram disulfide. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1764-1769.	0.2	2
3640	Crystal structure of 2,3,5,6-tetrakis(pyridin-2-yl)pyrazine hydrogen peroxide 4.75-solvate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1793-1796.	0.2	8
3641	Crystal structure of the Ba<sup>II</sup>-based Co<sup>II</sup>-containing one-dimensional coordination polymer poly[[aqua(1/4<sub>4</sub>-2,2<sup>2</sup>-[(4,10-dimethyl-1,4,7,10-tetraazacyclododecane-1,7-diyl)bis(methylidene)]bis(4-oxo-4 <i>H</i> -pyran-3-olato)]bis(perchlorate)]. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1806-1811.	0.2	2
3642	A new monoclinic polymorph of ( <i>N</i> )-(3-methylphenyl)ethoxycarbothioamide: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1889-1897.	0.2	10
3643	Decachlorocyclopentasilanes coordinated by pairs of chloride anions, with different cations, but the same solvent molecules. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1903-1907.	0.2	2
3644	Crystal structures of 2,6-dibromo-4-methylbenzonitrile and 2,6-dibromo-4-methylphenyl isocyanide. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1913-1916.	0.2	4
3645	Stoichiometric and polymorphic salt of imidazolium picrate monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1885-1888.	0.2	1
3646	Crystal structure of bis[1/42-2,2<sup>2</sup>-[(4,10-dimethyl-1,4,7,10-tetraazacyclododecane-1,7-diyl)bis(methylene)]bis(4-oxo-4 <i>H</i> -pyran-3-olato)]dicobaltcalcium bis(perchlorate) 1.36-hydrate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1959-1965.	0.2	1





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3683	Crystal structure, electrochemical and spectroscopic investigation of $\text{[Ru}(\text{tris}[\text{2}-(1\text{-H-imidazol-2-yl})\text{-3-pyrimidine}]\text{N}_3\text{]}(\text{PF}_6)_3 \cdot \text{H}_2\text{O}$ ruthenium(II) bis(hexafluoridophosphate) trihydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 874-877.	0.2	4
3684	Structure of copper(II) complexes grown from ionic liquids $\text{[1-ethyl-3-methylimidazolium acetate or chloride]}$ . <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 981-986.	0.2	7
3685	Crystal structure and Hirshfeld surface analysis of 4-[4-(1-H-benzodimidazol-2-yl)phenoxy]phthalonitrile monohydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 994-997.	0.2	7
3686	Crystal structure of 3,14-dimethyl-2,6,13,17-tetraazoniatricyclo[16.4.0.0.7.12]docosane tetrachloride tetrahydrate from synchrotron X-ray data. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1039-1041.	0.2	3
3687	The crystal structure of (E)-2-ethyl-N-(4-nitrobenzylidene)aniline: three-dimensional supramolecular assembly mediated by C-H...O hydrogen bonds and nitro... $\pi$ (arene) interactions. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1071-1074.	0.2	1
3688	Molecular structure, DFT studies and UV-Vis absorption of two new linear fused ring chalcones: (E)-1-(anthracen-9-yl)-3-(2-methoxyphenyl)prop-2-en-1-one and (E)-1-(anthracen-9-yl)-3-(3-fluoro-4-methoxyphenyl)prop-2-en-1-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1087-1092.	0.2	5
3689	Structural analysis of 2-iodobenzamide and 2-iodo-N-phenylbenzamide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1130-1133.	0.2	3
3690	Crystal structure of N-allyl-4-methylbenzenesulfonamide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1126-1129.	0.2	4
3691	Crystal structure and Hirshfeld surface analysis of 2,4-diamino-6-phenyl-1,3,5-triazin-1-ium 4-methylbenzenesulfonate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1159-1162.	0.2	2
3692	Crystal structure and Hirshfeld surface analysis of (E)-3-[(2,3-dichlorobenzylidene)amino]-5-phenylthiazolidin-2-iminium bromide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1168-1172.	0.2	11
3693	Hirshfeld surface analysis and crystal structure of 7-methoxy-5-methyl-2-phenyl-11,12-dihydro-5,11-methano-1,2,4-triazolo[1,5-c][1,3,5]benzoxadiazocine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1211-1214.	0.2	5
3694	Crystal structure and theoretical studies of two $\pi$ -conjugated fused-ring chalcones: (E)-1-(anthracen-9-yl)-3-(9-ethyl-9H-carbazol-3-yl)prop-2-en-1-one and (E)-1-(anthracen-9-yl)-3-[4-(9H-carbazol-9-yl)phenyl]prop-2-en-1-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1302-1308.	0.2	4
3695	Crystal structure and Hirshfeld surface analysis of (E)-5-phenyl-3-[(pyridin-4-ylmethylidene)amino]thiazolidin-2-iminium bromide monohydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1290-1294.	0.2	3
3696	Molecular and crystal structure of methyl 4-methyl-2,2-dioxo-1H-2,6,1-benzothiazine-3-carboxylate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1299-1301.	0.2	1
3697	Isomorphous diethyl 1-(4-chlorobenzyl)-4-(4-chlorophenyl)-2,2-dioxo-3,4,6,7,8,8a-hexahydro-1H-pyrrolo[2,1-c][1,4]thiazine-1,3-dicarboxylate and its 1-(4-methylbenzyl)-4-(4-methylphenyl)-substituted analogue obeying the chloro-methyl exchange rule. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1267-1271.	0.2	3
3698	Crystal structure of 2,3-bipyridine-2,6-dicarbonitrile. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1272-1275.	0.2	2
3699	A resonance-assisted intramolecular hydrogen bond in compounds containing 2-hydroxy-3,5-dinitrobenzoic acid and its various deprotonated forms: redetermination of several related structures. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1344-1357.	0.2	11
3700	Structural characterization and DFT study of bis{[(2-hydroxybenzyl)amino]-3-(4-hydroxyphenyl)propanoato}cadmium(II) tetrahydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1339-1343.	0.2	3



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3701	Crystal structure of 2-hydroxy-3-(prop-2-yn-1-yl)naphthalene-1,4-dione. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1319-1321.	0.2	1
3702	Crystal structure and Hirshfeld surface analysis of the 1:3 adduct of tetraaquatrinitratoneodymium(III) with 3-amino-1,2,4-triazine. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1309-1313.	0.2	2
3703	Crystal structure of the [(1,3-dimesityl-1H-imidazol-3-ium-2-yl)methanolato]copper(II) chloride dimer: insertion of formaldehyde into a copper $\pi$ -carbene bond. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1369-1372.	0.2	2
3704	Crystal structure and Hirshfeld surface analysis of (<i>E</i>)-1-(3,5-dichloro-2-hydroxyphenyl)-3-(5-methylfuran-2-yl)prop-2-en-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1451-1454.	0.2	9
3705	Structures of substituted pyridine <i>N</i>-oxide with manganese(II) acetate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1405-1410.	0.2	5
3706	Crystal structure and synthesis of 3-(1<i>H</i>-pyrrol-2-yl)-1-(thiophen-2-yl)propanone. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1463-1466.	0.2	1
3707	The crystal structure of bis{3,5-difluoro-2-[4-(2,4,6-trimethylphenyl)pyridin-2-yl]phenyl}(picolinato)iridium(III) and its 4-tert-butylpyridin-2-yl analogue. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1467-1470.	0.2	2
3708	Crystal structure of (<i>E</i>)-3-[(2,6-dimethylphenyl)diazenyl]-7-methyl-1<i>H</i>-indazole. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1421-1423.	0.2	3
3709	Crystal structure of 3,6-dihydroxy-4,5-dimethylbenzene-1,2-dicarbaldehyde. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1424-1426.	0.2	3
3710	Crystal structure and Hirshfeld surface analysis of 1,2-bis(2,6-diisopropoxy-[2,3-bipyridin]-6-yl)benzene. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1475-1479.	0.2	2
3711	Crystal structures, DFT studies and UV-visible absorption spectra of two anthracenyl chalcone derivatives. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1491-1496.	0.2	5
3712	Crystal structure and Hirshfeld surface analysis of (<i>E</i>)-<i>N</i>-[(2-ethoxynaphthalen-1-yl)methylidene]-5,6,7,8-tetrahydronaphthalen-1-amine. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1513-1516.	0.2	6
3713	Crystal structure, Hirshfeld surface analysis and HOMO-LUMO analysis of (<i>E</i>)-4-bromo-<i>N</i>-[(4-methoxybenzylidene)benzohydrazide]. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1500-1503.	0.2	6
3714	Investigation of solid-state photochemical nitro-nitrito linkage isomerization: crystal structures of <i>trans</i>-bis(ethylenediamine)(isothiocyanato)nitritocobalt(III) salts: thiocyanate, chloride monohydrate, and perchlorate-thiocyanate(0.75/0.25). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1526-1531.	0.2	5
3715	Crystal structure of (<i>E</i>)-2,6-dimethoxy-4-[(4-methoxyphenyl)imino]methylphenol. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1540-1542.	0.2	1
3716	Crystal structure of (diethyl) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 152 Td (ether- $\pi$ -O)[5,10,15,20-tetrakis(2-isothiocyanato)diethyl ether solvate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1609-1612.	0.2	2
3717	Crystal structure and metabolic activity of 4-(thien-2-yl)-2-methyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylic acid ethoxycarbonylphenylmethylester. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1577-1579.	0.2	4
3718	Crystal structure of the thalidomide analog (3a<i>R</i>*,7a<i>S</i>*)-2-(2,6-dioxopiperidin-3-yl)hexahydro-1<i>H</i>-isoindole-1,3(2<i>H</i>)-dione. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1595-1598.	0.2	1



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3719	Crystal structure and Hirshfeld surface analysis of 1-[[2-oxo-3-(prop-1-en-2-yl)-2,3-dihydro-1 <i>H</i> -1,3-benzodiazol-1-yl]methyl]-3-(prop-1-en-2-yl)-2,3-dihydro-1 <i>H</i> -1,3-benzodiazol-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1746-1750.	0.2	4
3720	Crystal structure and Hirshfeld surface analysis of (succinato- $\mu_2$ -O)[ $\mu_2$ -N,N',N'',N'''-tetrakis(2-hydroxyethyl)ethylenediamine- $\mu_2$ -5,5'-bis( $\mu_2$ -O,N,N',N''-tetrakis(2-hydroxyethyl)ethylenediamine)]nickel(II) tetrahydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1700-1704.	0.2	4
3721	Crystal structure of diaquatrakis(benzohydrazide- $\mu_2$ ) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 667 Td (N,N',O,O')(isophthalate)nickel(II) tetrahydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1691-1694.	0.2	2
3722	Two polymorphs of 2-(prop-2-yn-1-yloxy)naphthalene-1,4-dione: solvent-dependent crystallization. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1731-1734.	0.2	1
3723	Crystal structures of two hydrogen-bonded compounds of chloranilic acid-ethyleneurea (1/1) and chloranilic acid-hydantoin (1/2). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1727-1730.	0.2	3
3724	Binary charge-transfer complexes using pyromellitic acid dianhydride featuring C=H...O hydrogen bonds. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1772-1777.	0.2	4
3725	Four 1-aryl-1 <i>H</i> -pyrazole-3,4-dicarboxylate derivatives: synthesis, molecular conformation and hydrogen bonding. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1783-1789.	0.2	5
3726	Crystal structure and Hirshfeld surface analysis of 1-[(1-butyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl]-3-methylquinoxalin-2(1 <i>H</i> )-one. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1815-1820.	0.2	1
3727	A new co-crystal dinuclear/trinuclear Zn $^{II}$ /Zn $^{II}$ /Sm $^{III}$ /Zn $^{II}$ complex with a salen-type Schiff base ligand. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1862-1866.	0.2	6
3728	Crystal structure of 4-[(3-methoxy-2-oxidobenzylidene)azaniumyl]benzoic acid methanol monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1847-1850.	0.2	5
3729	Crystal structure and Hirshfeld surface analysis of (E)-2,4-di- <i>tert</i> -butyl-6-[(3-chloro-4-methylphenylimino)methyl]phenol. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1887-1890.	0.2	6
3730	Crystal structure, DFT calculations and Hirshfeld surface analysis of 3-(4-methylphenyl)-6-nitro-1 <i>H</i> -indazole. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1857-1861.	0.2	2
3731	Crystal structure and Hirshfeld surface analysis of two imidazo[1,2- <i>a</i> ]pyridine derivatives: <i>tert</i> -butyl-2-(4-methoxyphenyl)-5-methylimidazo[1,2- <i>a</i> ]pyridin-3-amine and <i>tert</i> -butyl-2-[4-(dimethylamino)phenyl]imidazo[1,2- <i>a</i> ]pyridin-3-amine. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1913-1918.	0.2	4
3732	Crystal structure of a 1:1 salt of 4-aminobenzoic acid (vitamin B <sub>10</sub> ) with pyrazinoic acid. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1923-1927.	0.2	6
3733	Crystal structure and Hirshfeld surface analysis of a new benzodiazepine derivative: 4-dichloromethyl-2,3-dihydro-1 <i>H</i> -1,5-benzodiazepin-2-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 33-37.	0.2	7
3734	Crystal structure of a second monoclinic polymorph of 3-methoxybenzoic acid with $Z = 1$ . Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 8-11.	0.2	1
3735	A 1:2 co-crystal of 2,2'-dithiodibenzoic acid and benzoic acid: crystal structure, Hirshfeld surface analysis and computational study. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1-7.	0.2	14
3736	The crystal structures of four dimethoxybenzaldehyde isomers. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 38-42.	0.2	1

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3737	Synthesis, crystal structure, DFT calculations and Hirshfeld surface analysis of 2-(1-decyl-2-oxoindolin-3-ylidene)propanedinitrile. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 21-25.	0.2	3
3738	Crystal structure, Hirshfeld surface analysis and DFT studies of (<i>E</i>)-1-(4-bromophenyl)-3-(3-fluorophenyl)prop-2-en-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 58-63.	0.2	8
3739	Crystal structure and Hirshfeld surface analysis of a chalcone derivative: (<i>E</i>)-3-(4-fluorophenyl)-1-(4-nitrophenyl)prop-2-en-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 53-57.	0.2	1
3740	Crystal structure of poly[[hexaaquatrakis(1/4-3,6-dioxocyclohexa-1,4-diene-1,4-diolato)dierbium(III)] octadecahydrate]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 64-67.	0.2	1
3741	Crystal structure and Hirshfeld surface analysis of (<i>N</i>)-2-[(<i>E</i>)-(4-methylbenzylidene)amino]phenyl)-2-(5-methyl-1-<i>H</i>-pyrazol-3-yl)acetamide hemihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 154-158.	0.2	8
3742	Crystal structure of a new 2,6-bis(imino)pyridine derivative: (1<i>E</i>)-1,1<i>E</i>-1,1<i>E</i>-2,6-diyl)bis[(<i>N</i>-4-chlorophenyl)ethan-1-imine]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 115-118.	0.2	1
3743	Synthesis, X-ray crystal structure, Hirshfeld surface analysis and DFT studies of (<i>E</i>)-(<i>N</i>-2-(2-bromobenzylidene)-4-methylbenzohydrazide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 109-114.	0.2	4
3744	Crystal structure of {2-methyl-2-[(pyridin-2-ylmethyl)amino]propan-1-ol- <sup>3</sup> }bis[nitrato- <sup>3</sup> o]copper(II) from synchrotron data. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 150-153.	0.2	1
3745	Crystal structure of 4-[(2-hydroxy-3-methoxybenzyl)amino]benzoic acid hemihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 159-162.	0.2	2
3746	Synthesis, crystal structure, spectroscopic features and Hirshfeld surfaces of 2-methyl-3-[(2-methylphenyl)carbamoyl]phenyl acetate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 423-427.	0.2	1
3747	Crystal structures of [IrCl <sub>2</sub> ](NHCHPh)((dppm)(C(N <sub>2</sub> dppm)) <sup>3</sup> ) Tj ETQq0.0.0 rgBT /Overlock 10 T	0.2	5
3748	fragmentation in a PCN pincer iridium complex. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 223-227.	0.2	5
3749	Sodium rubidium hydrogen citrate, NaRbHC <sub>6</sub> H <sub>5</sub> O <sub>7</sub> , and sodium caesium hydrogen citrate, NaCsHC <sub>6</sub> H <sub>5</sub> O <sub>7</sub> : crystal structures and DFT comparisons. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 292-298.	0.2	4
3750	Co-crystallization of 3,5-dinitrobenzoic acid with two antipsychotic agents: a simple 1:1 salt with trihexyphenidyl and a 1:2 acid salt containing a very short Oâ€”H...O hydrogen bond with chlorprothixene. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 292-298.	0.2	4
3751	Crystal structure of bromidopentakis(tetrahydrofuran- <sup>5</sup> o)magnesium bis[1,2-bis(diphenylphosphanyl)benzene- <sup>2</sup> ]-(<i>P</i>,<i>P</i>-1) cobaltate (&sup3;) tetrahydrofuran disolvate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 304-307.	0.2	1
3752	Crystal structure and Hirshfeld surface analysis of a Schiff base: (<i>Z</i>)-6-[(5-chloro-2-methoxyanilino)methylidene]-2-hydroxycyclohexa-2,4-dien-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 362-366.	0.2	4
3753	Crystal structure of potassium [4-amino-5-(benzo[<i>d</i>]thiazol-2-yl)-6-(methylsulfanyl)pyrimidin-2-yl](phenylsulfonyl)azanide dimethylformamide monosolvate hemihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 367-371.	0.2	10
3754	Synthesis and crystal structure of 2,4,6,8-tetrakis(3,5-di- <i>tert</i> -butylphenoxy)pyrimido[5,4- <i>d</i> ]pyrimidine: expansion of the Piedfort concept. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 383-387.	0.2	1
3755	Host-guest supramolecular interactions between a resorcinarene-based cavitand bearing a -COOH moiety and acetic acid. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 397-401.	0.2	2

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3755	Synthesis and crystal structure of 1,3-di- <i>tert</i> -butyl-2-chloro-4,4-diphenyl-1,3,2λ <sup>3</sup> ,4-diazaphosphasiletidine. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 405-409.	0.2	3
3756	Crystal structure of dilithium potassium citrate, Li <sub>2</sub> K <sub>6</sub> H <sub>5</sub> O <sub>7</sub> determined from powder diffraction data and DFT calculations. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 410-413.	0.2	3
3757	Sodium dirubidium citrate, NaRb <sub>2</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> , and sodium dirubidium citrate dihydrate, NaRb <sub>2</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> (H <sub>2</sub> O) <sub>2</sub> . Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 432-437.	0.2	3
3758	Crystal structure of NiFe(CO) <sub>5</sub> [tris(pyridylmethyl)azaphosphatane]: a synthetic mimic of the NiFe hydrogenase active site incorporating a pendant pyridine base. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 438-442.	0.2	4
3759	Crystal structure and Hirshfeld surface analysis of ( <i>E</i> )-1-(4-chlorophenyl)-2-[2,2-dichloro-1-(4-fluorophenyl)ethenyl]diazene. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 465-469.	0.2	16
3760	Crystal structure of diethyl 2-amino-5-[4-[bis(4-methylphenyl)amino]benzamido]thiophene-3,4-dicarboxylate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 589-592.	0.2	3
3761	Crystal structure of 1-heptafluorotolyl-closo-1,2-dicarbododecaborane. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 512-515.	0.2	1
3762	Crystal structure of memantine- <i>carboxyborane</i> . Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 543-546.	0.2	1
3763	Crystal structure of 4,5,6,7,8,8-hexachloro-2-(3,4-dimethoxyphenethyl)-3a,4,7,7a-tetrahydro-1 <i>H</i> -4,7-methanoisindole-1,3(2 <i>H</i> )-dione [+solvent]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 562-564.	0.2	1
3764	Comparison of the C-H...O bonding in two crystalline phases of 1,4-dithiane 1,1,4,4-tetraoxide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 576-579.	0.2	1
3765	Crystal structures and Hirshfeld surface analysis of 2-(adamantan-1-yl)-5-(4-fluorophenyl)-1,3,4-oxadiazole and 2-(adamantan-1-yl)-5-(4-chlorophenyl)-1,3,4-oxadiazole. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 611-615.	0.2	7
3766	Crystal structure and Hirshfeld surface analysis of <i>N</i> -(5-iodo-4-phenylthiazol-2-yl)acetamide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 717-720.	0.2	4
3767	( <i>E</i> )-1-(Benzo[ <i>d</i> ][1,3]dioxol-5-yl)-3-([2,2-bithiophen]-5-yl)prop-2-en-1-one: crystal structure, UV-Vis analysis and theoretical studies of a new <i>π</i> -conjugated chalcone. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 632-637.	0.2	3
3768	Bromination of bis(pyridin-2-yl) diselenide in methylene chloride: the reaction mechanism and crystal structures of 1 <i>H</i> -pyridine-2-selenenyl dibromide and its cycloadduct with cyclopentene (3 <i>a</i> <i>SR</i> ,9 <i>a</i> <i>RS</i> )-2,3,3 <i>a</i> ,9 <i>a</i> -tetrahydro-1 <i>H</i> -cyclopenta[4,5][1,3]selenazolo[3,2- <i>a</i> ]pyridinium bromide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 675-679.	0.2	6
3769	Crystal structure and Hirshfeld surface analysis of ( <i>rac</i> )-2-[2-(4-chlorophenyl)-3,4-dihydro-2 <i>H</i> -1-benzopyran-4-ylidene]hydrazine-1-carbothioamide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 707-710.	0.2	1
3770	Crystal structure and Hirshfeld surface analysis of 4-(2,6-dichlorobenzyl)-6-phenylpyridazin-3(2 <i>H</i> )-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 650-654.	0.2	2
3771	Crystal structure and Hirshfeld surface analysis of (1/4-2-[4-[(carboxylatomethyl)carbamoyl]benzamido]acetato) <sup>2-</sup> Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 107 Td ( <i>O</i> )- <i>N,N,N'</i> , <i>N'</i> -1,4-phenylenedicarbonyldiglycine monosolvate octahydrate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 667-674.	0.2	9
3772	Crystal structure and optical properties of fused-ring chalcone ( <i>E</i> )-3-(anthracen-9-yl)-1-(4-nitrophenyl)prop-2-en-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 685-689.	0.2	5

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3773	Crystal structure and Hirshfeld surface analysis of dibutyl 5,5- $\epsilon^2$ -(pentane-3,3-diyl)bis(1 <i>H</i> -pyrrole-5-carboxylate). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 711-713.	0.2	6
3774	Crystal structure of 1-anilino-5-methyl-1 <i>H</i> -1,2,3-triazole-4-carboxylic acid monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 738-741.	0.2	4
3775	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of 3- $\{2$ - $\{2$ -(2,4-dichlorophenyl)methylidene $\}$ -3-oxo-3,4-dihydro-2 <i>H</i> -1,4-benzothiazin-4-yl $\}$ propanenitrile. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 721-727.	0.2	12
3776	Crystal structure and Hirshfeld surface analysis of ( <i>E</i> )-2-(2,4,6-trimethylbenzylidene)-3,4-dihydronaphthalen-1( <i>H</i> )-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 746-750.	0.2	8
3777	Crystal structure of bis(4-methoxypyridine- <i>N</i> )( <i>meso</i> -5,10,15,20-tetraphenylporphyrinato- $\text{I}^{\text{9}}$ ) Tj ETQq0 0 0 r gBT /Overlock 10 Tf	0.2	1
3778	Crystal structure of pifenidone (5-methyl-1-phenyl-1 <i>H</i> -pyridin-2-one): an active pharmaceutical ingredient (API). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 984-986.	0.2	6
3779	Crystal structure and DFT study of ( <i>E</i> )-2-chloro-4- $\{2$ -(2,4-dinitrophenyl)hydrazin-1-ylidene $\}$ methylphenol acetonitrile hemisolvate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 770-773.	0.2	4
3780	Crystal structure and Hirshfeld surface analysis of a conformationally unsymmetrical bischalcone: (1 <i>E</i> ,4 <i>E</i> )-1,5-bis(4-bromophenyl)penta-1,4-dien-3-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 774-779.	0.2	5
3781	Crystal structure, Hirshfeld surface analysis and HOMO-LUMO analysis of ( <i>E</i> )- <i>N</i> - $\epsilon^2$ -(3-hydroxy-4-methoxybenzylidene)nicotinohydrazide monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 804-807.	0.2	5
3782	Crystal structure and Hirshfeld surface analysis of ( <i>Z</i> )-6- $\{2$ -(2-hydroxy-4-methylanilino)methylidene $\}$ -4-methylcyclohexa-2,4-dien-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 785-788.	0.2	1
3783	Crystal structures and Hirshfeld surface analyses of 4,4- $\epsilon^2$ - $\{1,3$ -phenylenebis(methylene) $\}$ bis(oxy) $\}$ bis(3-methoxybenzaldehyde) and		





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3809	Crystal structure and Hirshfeld surface analysis of 2-[(2-oxo-2 <i>H</i> -chromen-4-yl)oxy]acetic acid dimethyl sulfoxide monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1123-1127.	0.2	1
3810	Syntheses, crystal structures and Hirshfeld surface analyses of (3 <i>a</i> - <i>R</i> ,4 <i>i</i> - <i>S</i> ,7 <i>i</i> - <i>R</i> ,7 <i>a</i> - <i>S</i> )-2-(perfluoropyridin-4-yl)-3 <i>a</i> ,4,7,7 <i>a</i> -tetrahydro-4,7-methanoisindole-1,3-dione and (3 <i>a</i> - <i>R</i> ,4 <i>i</i> - <i>S</i> ,7 <i>i</i> - <i>R</i> ,7 <i>a</i> - <i>S</i> )-2-[(perfluoropyridin-4-yl)oxy]-3 <i>a</i> ,4,7,7 <i>a</i> -tetrahydro-4,7-methanoisindole-1,3-dione. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1153-1157.	0.2	4
3811	Crystal structure of 4,4- $\epsilon^2$ -bis(4-bromophenyl)-1,1- $\epsilon^2$ ,3,3- $\epsilon^2$ -tetrathiafulvalene. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1195-1198.	0.2	1
3812	Crystal structures of an imidazo[1,5- <i>a</i> ]pyridinium-based ligand and its (C <sub>13</sub> H <sub>12</sub> N <sub>3</sub> ) <sub>2</sub> [Cd <sub>4</sub> ] hybrid salt. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1209-1214.	0.2	4
3813	Crystal structures and Hirshfeld surface analyses of the two isotopic compounds ( <i>E</i> )-1-(4-bromophenyl)-2-[2,2-dichloro-1-(4-nitrophenyl)ethenyl]diazene and ( <i>E</i> )-1-(4-chlorophenyl)-2-[2,2-dichloro-1-(4-nitrophenyl)ethenyl]diazene. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1199-1204.	0.2	12
3814	Crystal structure of tetra- $\frac{1}{4}$ -acetato-bis[(5-amino-2-methylsulfanyl-1,3,4-thiadiazole- <i>N</i> ) Tj ETQq1 1 0.784314 rgBT /Overlock 10 1239-1242.	0.2	3
3815	Syntheses and crystal structures of a new family of hybrid perovskites: C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> · <i>A</i> Br <sub>3</sub> ·0.5H <sub>2</sub> O ( <i>A</i> = K, Tj ETQq0 0 0 rgBT /Overlock 10 1239-1242).	0.2	0
3816	Crystal structures of two isomeric 2-aryl-3-phenyl-1,3-thiazepan-4-ones. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1270-1273.	0.2	2
3817	Crystal structure and Hirshfeld surface analysis of bis(benzoato- $\epsilon^2$ ) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 427 Td ( <i>O</i> ) Crystallographic Communications, 2019, 75, 1301-1305.	0.2	2
3818	Crystal structure, Hirshfeld surface analysis and computational studies of 5-[(prop-2-en-1-yl)sulfanyl]-1-[2-(trifluoromethyl)phenyl]-1 <i>H</i> -tetrazole. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1331-1335.	0.2	1
3819	Synthesis and redetermination of the crystal structure of salicylaldehyde ( <i>N</i> )-(4-morpholiniothiosemicarbazone. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1389-1393.	0.2	6
3820	The synthesis and crystal structure of bis[3,3-diethyl-1-(phenylimino- $\epsilon^2$ )thiourea- <i>S</i> ]silver hexafluoridophosphate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1394-1398.	0.2	3
3821	Crystal structure of (1 <i>S</i> ,2 <i>R</i> )-2-[(3 <i>R</i> ,4 <i>S</i> )-3-methyl-4-phenyl-1,2,3,4-tetrahydroisoquinolin-2-yl]-1,2-diphenylethan-1-ol. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1399-1402.	0.2	4
3822	The structure and Hirshfeld surface analysis of the salt 3-methacrylamido- <i>N</i> , <i>N</i> , <i>N</i> -trimethylpropan-1-aminium 2-acrylamido-2-methylpropane-1-sulfonate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1403-1410.	0.2	1
3823	Crystal structures and Hirshfeld surface analyses of ( <i>E</i> )- <i>N</i> - $\epsilon^2$ -benzylidene-2-oxo-2 <i>H</i> -chromene-3-carbohydrazide and the disordered hemi-DMSO solvate of ( <i>E</i> )-2-oxo- <i>N</i> - $\epsilon^2$ -(3,4,5-trimethoxybenzylidene)-2 <i>H</i> -chromene-3-carbohydrazide: lattice energy and intermolecular interaction energy calculations for the former. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1403-1410.	0.2	3
3824	Crystal structure and Hirshfeld surface analysis of 2-hydroxy-7-methoxy-1,8-bis(2,4,6-trichlorobenzoyl)naphthalene. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1418-1422.	0.2	3
3825	Crystal structure and Hirshfeld surface analysis of ( <i>N</i> )-(tert-butyl)-2-(phenylethynyl)imidazo[1,2- <i>a</i> ]pyridin-3-amine. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1564-1567.	0.2	2
3826	Crystal structure and Hirshfeld surface analysis of 2-aminopyridinium hydrogen phthalate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1627-1631.	0.2	3



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3827	Crystal structure of tetrakis(tetrahydrofuran- $\eta^5$ -O)bis(trifluoromethanesulfonato- $\eta^5$ -O)iron(II). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1548-1551.	0.2	1
3828	Crystal structure and DFT study of a zinc xanthate complex. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1582-1585.	0.2	4
3829	Crystal structures of two charge-transfer complexes of benzo[1,2-c:3,4-c' $\rightarrow$ 5,6-c'' $\rightarrow$ 2]trithiophene ( <i>D</i> <sub>3h</sub> -BTT). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1573-1577.	0.2	3
3830	Crystal structure, DFT calculation, Hirshfeld surface analysis and energy framework study of 6-bromo-2-(4-bromophenyl)imidazo[1,2-a]pyridine. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1620-1626.	0.2	15
3831	Bis[2-(4,5-diphenyl-1H-imidazol-2-yl)-4-nitrophenolato]copper(II) dihydrate: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1664-1671.	0.2	1
3832	Crystal structure, synthesis and thermal properties of bis(acetonitrile- $\eta^5$ -N)bis(4-benzoylpyridine- $\eta^5$ -N)bis(isothiocyanato- $\eta^5$ -N)nickel(II). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1685-1688.	0.2	4
3833	The first structural characterization of the protonated azacyclam ligand in <i>catena</i> -poly[[[(perchlorato)copper(II)]- $\eta^4$ -3-(3-carboxypropyl)-1,5,8,12-tetraaza-3-azoniacyclotetradecane]bis(perchlorate)]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1700-1704.	0.2	1
3834	Crystal structure and Hirshfeld surface analysis of 2-(4-nitrophenyl)-2-oxoethyl benzoate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1719-1723.	0.2	3
3835	Crystal structures of two dimeric nickel diphenylacetate complexes. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1768-1773.	0.2	2
3836	Crystal structure and Hirshfeld surface analysis of 2-(4-nitrophenyl)-2-oxoethyl picolinate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1763-1767.	0.2	3
3837	Crystal structure of benzo[ <i>h</i> ]quinoline-3-carboxamide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1828-1832.	0.2	2
3838	Crystal structure of 4,6-dimethyl-2-[(2,3,4,6-tetra-O-acetyl- $\beta$ -D-galactopyranosyl)sulfanyl]pyrimidine. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1820-1823.	0.2	6
3839	Some reflections on symmetry: pitfalls of automation and some illustrative examples. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1812-1819.	0.2	11
3840	Crystal structure and Hirshfeld surface analysis of a zinc xanthate complex containing the 2,2'-bipyridine ligand. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1857-1860.	0.2	3
3841	Crystal structure, Hirshfeld surface analysis and DFT studies of 6-[( <i>E</i> )-2-(thiophen-2-yl)ethenyl]-4,5-dihydropyridazin-3( <i>H</i> )-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1880-1883.	0.2	8
3842	Crystal and molecular structure of jatrophane diterpenoid (2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>R</i> ,7 <i>S</i> ,8 <i>S</i> ,9 <i>S</i> ,13 <i>S</i> ,14 <i>S</i> ,15 <i>R</i> )-2,3,9-triacetoxy-5,14-dihydro-1 <i>H</i> -jatropha-1,4-dione. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1884-1887.	0.2	3
3843	Crystal structures of ( <i>E</i> )-3-(4-hydroxybenzylidene)chroman-4-one and ( <i>E</i> )-3-(3-hydroxybenzylidene)-2-phenylchroman-4-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1907-1913.	0.2	2
3844	Crystal structure, Hirshfeld analysis and a molecular 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-oxadiazol-3-yl]methyl]-2 <i>H</i> -1,2,6-thiadiazine-4-carboxylate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 12-17.	0.2	2

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3845	<i>checkCIF</i> validation ALERTS: what they mean and how to respond. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1-11.	0.2	769
3846	Crystal structure of the coordination polymer <i>catena</i>-poly[[[(acetonitrile- $\lambda^5$ -N)copper(II)] $\frac{1}{4}$ -1,3-dithiolane- $\lambda^6$ ] $\frac{3}{4}$ hexafluorodiphosphate]. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 38-41.	0.2	5
3847	Syntheses and crystal structures of three [M(acac) $_2$ (TMEDA)] complexes (M = Tj, ET, Q, Q0, Q1, Q2, Q3, Q4, Q5, Q6, Q7, Q8, Q9, Rg, BT, Q, Overlock, 10)	0.2	6
3848	Crystal structure and Hirshfeld surface analysis of (<i>E</i>)-3-(3-iodophenyl)-1-(4-iodophenyl)prop-2-en-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 72-76.	0.2	3
3849	An unusually short intermolecular Nâ€”H...N hydrogen bond in crystals of the hemi-hydrochloride salt of 1-(<i>exo</i>-acetamidopyrrolizidine. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 77-81.	0.2	2
3850	Crystal structure, DFT and Hirshfeld surface analysis of (<i>E</i>)-N-[(1-chloro-3,4-dihydronaphthalen-2-yl)methylidene]benzohydrazide monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 132-136.	0.2	21
3851	Crystal structure, spectroscopic characterization and Hirshfeld surface analysis of aquadichlorido-N-[(pyridin-2-yl)methylidene]aniline)copper(II) monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 148-154.	0.2	5
3852	Crystal structure, DFT and MEP study of (<i>E</i>)-2-[(3-chlorophenyl)imino]methyl-6-methylphenol. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 141-144.	0.2	7
3853	Synthesis, crystal structure and spectroscopic and Hirshfeld surface analysis of 4-hydroxy-3-methoxy-5-nitrobenzaldehyde. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 239-244.	0.2	5
3854	The synthesis, crystal structure and Hirshfeld analysis of 4-(3,4-dimethylanilino)-N-(3,4-dimethylphenyl)quinoline-3-carboxamide. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 201-207.	0.2	2
3855	Crystal structure of 4-methyl-N-(4-methylbenzyl)benzenesulfonamide. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 235-238.	0.2	1
3856	Crystal structure of 2-methyl-1,2,3,4-tetrahydroisoquinoline trihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 298-302.	0.2	4
3857	Synthesis and crystal structure of (2S,4aR,8aR)-6-oxo-2,4a,6,8a-tetrahydropyrano[3,2-b]pyran-2-carboxamide. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 761-764.	0.2	1
3858	Crystal structure of 1,4,8,11-tetramethyl-1,4,8,11-tetraazoniacyclotetradecane bis(perchlorate) dichloride from synchrotron X-ray data. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 324-327.	0.2	4
3859	Crystal structure of imidazo[1,5-a]pyridinium-based hybrid salt (C $_{13}$ H $_{12}$ N $_3$ ) $_2$ [MnCl $_4$ ]. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 309-313.	0.2	2
3860	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of 1-(1,3-benzothiazol-2-yl)-3-(2-hydroxyethyl)imidazolidin-2-one. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 370-376.	0.2	1
3861	Conversion of diarylchalcones into 4,5-dihydropyrazole-1-carbothioamides: molecular and supramolecular structures of two precursors and three products. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 360-365.	0.2	4
3862	Phosphorescent mono- and diiridium(III) complexes cyclometalated by fluorenyl- or phenyl-pyridino ligands with bulky substituents, as prospective OLED dopants. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 392-399.	0.2	3

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3863	Crystal structure of (<i>R</i>)-5-[(<i>R</i>)-3-(4-chlorophenyl)-5-methyl-4,5-dihydroisoxazol-5-yl]-2-methylcyclohex-2-enone. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 400-403.	0.2	8
3864	Crystal structure of 1-[(4-methylbenzene)sulfonyl]pyrrolidine. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 452-455.	0.2	1
3865	Crystal structure of 2-[bis(benzylsulfonyl)methyl]-6-methoxyphenol. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 484-487.	0.2	1
3866	Whole-molecule disorder of the Schiff base compound 4-chloro-<i>N</i>-[(4-nitrobenzylidene)aniline: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 417-422.	0.2	3
3867	Syntheses and crystal structures of the one-dimensional coordination polymers formed by [Ni(cyclam)] <sup>2+</sup> cations and 1,3-bis(3-carboxypropyl)tetramethyldisiloxane anions in different degrees of deprotonation. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 446-451.	0.2	2
3868	Polymorphism of 2-(5-benzyl-6-oxo-3-phenyl-1,6-dihydropyridazin-1-yl)acetic acid with two monoclinic modifications: crystal structures and Hirshfeld surface analyses. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 432-437.	0.2	3
3869	Synthesis and crystal structure of (1,4,7,10-tetraazacyclododecane- $\hat{\eta}^4$ ) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 507 Td (<i>N</i>). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 456-460.	0.2	1
3870	Crystal structure of ethyl 2-(5-amino-1-benzenesulfonyl-3-oxo-2,3-dihydro-1<i>H</i>-pyrazol-2-yl)acetate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 481-483.	0.2	6
3871	Crystal structure and Hirshfeld surface analysis of (C <sub>7</sub> H <sub>9</sub> N <sub>4</sub> O <sub>2</sub> )[ZnCl <sub>3</sub> (H <sub>2</sub> O)]. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 506-509.	0.2	2
3872	A redetermination of the crystal structure of the mannitol complex NH <sub>4</sub> [Mo <sub>2</sub> O <sub>5</sub> (C <sub>6</sub> H <sub>11</sub> O <sub>6</sub> ) $\hat{A}$ H <sub>2</sub> O] $\cdot$ 3H <sub>2</sub> O. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 518-522.	0.2	3
3873	Crystal structure, Hirshfeld surface analysis and computational study of 2-chloro-<i>N</i>-[4-(methylsulfonyl)phenyl]acetamide. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 594-598.	0.2	8
3874	The first coordination compound of 6-fluoronicotinate: the crystal structure of a one-dimensional nickel(II) coordination polymer containing the mixed ligands 6-fluoronicotinate and 4,4'-bipyridine. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 500-505.	0.2	4
3875	Crystal structure of 1,4,8,11-tetramethyl-1,4,8,11-tetraazoniacyclotetradecane bis[chloridochromate(VI)] dichloride from synchrotron X-ray data. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 523-526.	0.2	2
3876	Synthesis and crystal structures of two 1,3-di(alkyloxy)-2-(methylsulfonyl)imidazolium tetrafluoroborates. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 552-556.	0.2	1
3877	Crystal structures of <i>trans</i>-acetyldicarbonyl( $\hat{\eta}^5$ -cyclopentadienyl)(1,3,5-triaza-7-phosphaadamantane)molybdenum(II) and <i>trans</i>-acetyldicarbonyl( $\hat{\eta}^5$ -cyclopentadienyl)(3,7-diacetyl-1,3,7-triaza-5-phosphabicyclo[3.3.1]nonane)molybdenum(II). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 547-551.	0.2	2
3878	Structural investigation of methyl 3-(4-fluorobenzoyl)-7-methyl-2-phenylindolizine-1-carboxylate, an inhibitory drug towards <i>Mycobacterium tuberculosis</i>. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 567-571.	0.2	5
3879	Norpsilocin: freebase and fumarate salt. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 589-593.	0.2	11
3880	Crystal structures of ( $\hat{\eta}^4$ -cycloocta-1,5-diene)bis(1,3-dimethylimidazol-2-ylidene)iridium(I) iodide and ( $\hat{\eta}^4$ -cycloocta-1,5-diene)bis(1,3-diethylimidazol-2-ylidene)iridium(I) iodide. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 611-614.	0.2	2

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3881	Crystal structure and Hirshfeld surface analysis of diethyl 5-(2-cyanophenoxy)isophthalate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 905-908.	0.2	3
3882	Synthesis, crystal structure, DFT calculations and Hirshfeld surface analysis of 3-butyl-2,6-bis(4-fluorophenyl)piperidin-4-one. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 651-655.	0.2	17
3883	Crystal structure of $N,N$ -[4-(dimethylamino)benzylidene]furan-2-carbohydrazide monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 660-663.	0.2	3
3884	<i>Cis</i> versus <i>trans</i> arrangement of dithiocarbazate ligands in bis-chelated Ni and Cu complexes. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 692-696.	0.2	4
3885	Obtaining the best results: aspects of data collection, model finalization and interpretation of results in small-molecule crystal-structure determination. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 765-775.	0.2	9
3886	Crystal structure and Hirshfeld surface analysis of 6-benzoyl-3,5-diphenylcyclohex-2-en-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 720-723.	0.2	15
3887	A five-coordinate cobalt bis(dithiolene)phosphine complex [Co(pdt) <sub>2</sub> (PTA)] (pdt = Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Crystallographic Communications, 2020, 76, 736-741.	0.2	3
3888	Hydrogen-bonding patterns in 2,2-bis(4-methylphenyl)hexafluoropropane pyridinium and ethylenediammonium salt crystals. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 742-746.	0.2	2
3889	Crystal structure and Hirshfeld surface analysis of 4-{2,2-dichloro-1-[(4-fluorophenyl)diazenyl]ethenyl}- <i>N,N</i> -dimethylaniline. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 811-815.	0.2	7
3890	Molecular and crystal structure, lattice energy and DFT calculations of two 2-(nitrobenzoyloxy)acetophenone isomers. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 857-861.	0.2	3
3891	Crystal structure of the one-dimensional coordination polymer formed by the macrocyclic [Ni(cyclam)] <sup>2+</sup> cation and the dianion of diphenylsilanediylbis(4-benzoic acid). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 929-932.	0.2	1
3892	Crystal structure and Hirshfeld surface analysis of 4-(naphthalen-2-yl)- <i>N,N</i> -[( <i>Z</i> )-4-propoxybenzylidene]-1,3-thiazol-2-amine. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 920-923.	0.2	2
3893	Crystal structure of (1,4-diphenyl-4- <i>H</i> -1,2,4-triazol-3-yl)phenylamine difluorophosphate, and a survey of the difluorophosphate anion (PO <sub>2</sub> F <sub>2</sub> ) <sup>-</sup> . Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1003-1006.	0.2	2
3894	Crystal structure and Hirshfeld surface analysis of 4-bromoanilinium nitrate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 973-976.	0.2	4
3895	Crystal structures of three platinacyclic complexes bearing isopropyl eugenoxycetate and pyridine derivatives. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1012-1017.	0.2	3
3896	Synthesis and crystal structure of [Zn <sub>6</sub> Br <sub>4</sub> (C <sub>9</sub> H <sub>18</sub> NO) <sub>4</sub> (OH) <sub>4</sub> ] $\cdot$ 2C <sub>3</sub> H <sub>6</sub> O. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 998-1002.		
3897	Crystal structure, Hirshfeld surface analysis and computational study of a rhodamine Bsalicylaldehyde Schiff base derivative. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1027-1032.	0.2	5
3898	Phenol hemihydrate: redetermination of the crystal structure by neutron powder diffraction, Hirshfeld surface analysis and characterization of the thermal expansion. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1062-1069.	0.2	1

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3899	Crystal structure of 4-methyl-N-propylbenzenesulfonamide. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1070-1074.	0.2	3
3900	Crystal structures of two heterotrimetallic dysprosium-manganese-sodium 12-metallacrown-4 complexes with the bridging ligands 3-hydroxybenzoate and 4-hydroxybenzoate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1213-1221.	0.2	3
3901	One molecule, three crystal structures: conformational trimorphism of N-[(1S)-1-phenylethyl]benzamide. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1229-1233.	0.2	3
3902	A solid solution of ethyl and <i>d</i> -methyl 2-[(4-methylpyridin-2-yl)amino]-4-(pyridin-2-yl)thiazole-5-carboxylate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1255-1259.	0.2	2
3903	Crystal structure and Hirshfeld surface analysis of the product of the ring-opening reaction of a dihydrobenzoxazine: 6,6'-[(cyclohexylazanediy)bis(methylene)]bis(2,4-dimethylphenol). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1239-1244.	0.2	3
3904	Crystal structure and Hirshfeld surface analysis of (E)-4-[2,2-dichloro-1-[(3,5-dimethylphenyl)diazanyl]ethenyl]-N,N-dimethylaniline. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1251-1254.	0.2	8
3905	Synthesis, crystal structure and Hirshfeld surface of bis(2-aminopyridinium) hexachloridostannate(IV). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1279-1283.	0.2	5
3906	(E)-1-(2,6-Dichlorophenyl)-2-(3-nitrobenzylidene)hydrazine: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1291-1295.	0.2	2
3907	Hexaaquanickel(II) bis[triaqua- $\lambda$ -oxalato-di- $\lambda$ -oxalato-bariumchromate(III)] tetrahydrate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1316-1319.	0.2	1
3908	Piperidinium-2-carboxylate bis(hydrogen peroxide): unusual hydrogen-bonded peroxide chains. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1331-1335.	0.2	8
3909	Crystal structure of zwitterionic 3,3'-[1,1'-butane-1,4-diyl]bis(1H-imidazol-3-ium-3,1-diyl)]bis(propane-1-sulfonate) dihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1353-1356.	0.2	2
3910	Crystal structure and Hirshfeld surface analysis of phenyl(5,7,8a-triphenyl-1,2,3,7,8,8a-hexahydroimidazo[1,2-a]pyridin-6-yl)methanone with an unknown solvent. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1365-1368.	0.2	3
3911	Crystal structure of (1S,2S,3S)-1-benzoyl-2-(4-methoxyphenyl)-1-methyl-2,5,6,10-tetrahydro-1H-imidazo[1,2-a]pyridin-6-ylmethanone. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1548-1550.	0.2	1
3912	[2-Chloro-3-nitro-5-(trifluoromethyl)phenyl](piperidin-1-yl)methanone: structural characterization of a side product in benzothiazinone synthesis. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1442-1446.	0.2	2
3913	Crystal structures of three anionic lanthanide-aluminium [3.3.1] metallacryptate complexes. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1458-1466.	0.2	3
3914	Crystal structures of tolfenamic acid polymorphic forms I and II with precise hydrogen-atom positions for nuclear magnetic resonance studies. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1421-1426.	0.2	5
3915	Crystal structure of dichlorido- $\lambda$ -1,2'-bis(chloro)- $\lambda$ -3,5-dimethyl-1H-pyrazolato-1H-imidazo[1,2-a]pyridin-6-ylmethanone. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1503-1507.	0.2	3
3916	Formation of a nonanuclear copper(II) cluster with 3,5-dimethylpyrazolate starting from an NHC complex of copper(I) chloride. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1486-1490.	0.2	2



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3917	Crystal structure and Hirshfeld surface analysis of (aqua- $\lambda^5$ -O)(methanol- $\lambda^5$ -O)[ $\lambda^5$ -N-(2-oxidobenzylidene)threoninato- $\lambda^3$ ] $\lambda^5$ -copper(II). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1539-1542.	0.2	6
3918	Crystal structures of three functionalized chalcones: 4-dimethylamino-3-nitrochalcone, 3-dimethylamino-3-nitrochalcone and 3-nitrochalcone. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1599-1604.	0.2	3
3919	Crystal structures of two magnesium citrates from powder diffraction data. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1611-1616.	0.2	5
3920	Crystal structure, optical property and Hirshfeld surface analysis of bis[1-(prop-2-en-1-yl)-1H-imidazol-3-ium] hexachloridostannate(IV). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1624-1628.	0.2	7
3921	Crystal structures of monohydrate and methanol solvate compounds of {1-[(3,5-bis{[(4,6-dimethylpyridin-2-yl)amino]methyl}-2,4,6-triethylbenzyl)amino]cyclopentyl}methanol. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1679-1683.	0.2	6
3922	Crystal structure of $\lambda^5$ -bis[(1-benzyl-1H-1,2,3-triazol-4-yl)methylidene]-2,2-dimethylpropane-1,3-diamine}bis(thiocyanato- $\lambda^5$ -N)iron(III). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1661-1664.		
3923	Crystal structure of aqua(citric acid)(hydrogen citrate)calcium monohydrate, [Ca(HC <sub>6</sub> H <sub>5</sub> O <sub>7</sub> )(H <sub>3</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> )(H <sub>2</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> )(H <sub>2</sub> O) <sub>3</sub> ]. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1693-1698.	0.2	3
3924	Crystal structure of aqua(citric acid)(hydrogen citrate)calcium monohydrate, [Ca(HC <sub>6</sub> H <sub>5</sub> O <sub>7</sub> )(H <sub>3</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> )(H <sub>2</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> )(H <sub>2</sub> O) <sub>3</sub> ]. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1693-1698.	0.2	3
3925	Crystal structure of (N <sup>+</sup> C) cyclometalated Au <sup>III</sup> diazide at 100 Å...K. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1725-1727.	0.2	4
3926	Crystal structure and Hirshfeld surface analysis of dichlorido(methanol- $\lambda^5$ -O)bis(2-methylpyridine- $\lambda^5$ -N)copper(II). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1771-1774.	0.2	1
3927	Structure of tetrakis( $\lambda^5$ -decanoato- $\lambda^2$ )Tj ETQqO O 0 rgBT /Overlock 10 Tf 50 347 Td ( $\lambda^5$ -O):( $\lambda^5$ -O) $\lambda^5$ -bis[(4-methylpyridin-2-yl)amino]cyclopentyl}methanol. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1775-1778.	0.2	1
3928	Crystal structure and Hirshfeld surface analysis of a third polymorph of 2,6-dimethoxybenzoic acid. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1823-1826.	0.2	2
3929	Crystal structure of a new hydrate form of the NSAID sodium diclofenac. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1846-1850.	0.2	1
3930	Using more than 801 296 small-molecule crystal structures to aid in protein structure refinement and analysis. Acta Crystallographica Section D: Structural Biology, 2017, 73, 234-239.	1.1	6
3931	Ligand fitting with CCP4. Acta Crystallographica Section D: Structural Biology, 2017, 73, 158-170.	1.1	18
3932	Validation and extraction of molecular-geometry information from small-molecule databases. Acta Crystallographica Section D: Structural Biology, 2017, 73, 103-111.	1.1	19
3933	Iron-sulfur clusters have no right angles. Acta Crystallographica Section D: Structural Biology, 2019, 75, 16-20.	1.1	16
3934	Design guidelines for an electron diffractometer for structural chemistry and structural biology. Acta Crystallographica Section D: Structural Biology, 2019, 75, 458-466.	1.1	12



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3935	Crystal structures and snapshots along the reaction pathway of human phosphoserine phosphatase. <i>Acta Crystallographica Section D: Structural Biology</i> , 2019, 75, 592-604.	1.1	11
3936	Improved chemistry restraints for crystallographic refinement by integrating the Amber force field into <i>Phenix</i> . <i>Acta Crystallographica Section D: Structural Biology</i> , 2020, 76, 51-62.	1.1	29
3937	A new modulated crystal structure of the ANS complex of the St John's wort Hyp-1 protein with 36 protein molecules in the asymmetric unit of the supercell. <i>Acta Crystallographica Section D: Structural Biology</i> , 2020, 76, 653-667.	1.1	2
3938	1,2,3,5-Tetramethyl-1H-pyrazol-2-ium triiodide. <i>IUCrData</i> , 2016, 1, .	0.1	2
3939	Redetermination of diaqua[N,N'-bis(3-methoxy-2-oxidobenzylidene)ethylenediamine- $\eta^4$ O,N,N'- $\eta^2$ ,O $\eta^2$ ]manganese(III) perchlorate $\cdot$ 100H $_2$ O. <i>IUCrData</i> , 2016, 1, .	0.1	1
3940	Ferrocenecarboxylic anhydride: a redetermination. <i>IUCrData</i> , 2016, 1, .	0.1	1
3941	1,1'-bis-(Diphosphene-1,2-diyl)bis(2,2,6,6-tetramethylpiperidine). <i>IUCrData</i> , 2017, 2, .	0.1	2
3942	3,5-Dibromobenzonitrile. <i>IUCrData</i> , 2018, 3, .	0.1	1
3943	N,N'-Bis(4-bromophenyl)-N,N'-dimethylurea. <i>IUCrData</i> , 2018, 3, .	0.1	1
3944	1,3-Bis(4-bromophenyl)propane. <i>IUCrData</i> , 2018, 3, .	0.1	2
3945	Diisopropylammonium hydrogen phthalate. <i>IUCrData</i> , 2018, 3, .	0.1	2
3946	Betaine (trimethylammonioacetate) binary compound with sodium iodide. <i>IUCrData</i> , 2018, 3, .	0.1	1
3947	Revision of the crystal structure of 'bis(glycine) squaric acid'. <i>IUCrData</i> , 2018, 3, .	0.1	1
3948	Bis(pyrrrolidinium) hexachloridostannate: a redetermination. <i>IUCrData</i> , 2018, 3, .	0.1	1
3949	( <i>Z</i> )-1,2-Bis(3-bromophenyl)diazene 1-oxide. <i>IUCrData</i> , 2018, 3, .	0.1	1
3950	1-Methyl-4-thiocarbamoylpyridin-1-ium iodide. <i>IUCrData</i> , 2018, 3, .	0.1	1
3951	Polar crystal of vanillylformamide through replacement of the alkene by an isosteric formamide group. <i>IUCrData</i> , 2018, 3, .	0.1	2
3952	Construction of a supramolecule comprising [2,3,9,10,16,17,23,24-octakis(2,6-dimethylphenoxy)phthalocyaninato]zinc(II) and (5,10,15,20-tetraphenylporphyrinato)zinc(II). <i>IUCrData</i> , 2018, 3, .	0.1	1

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3953	1-Methyl-1 <i>H</i> -imidazol-3-ium methanesulfonate. IUCrData, 2018, 3, .	0.1	3
3954	Dibromidobis(3-bromobenzyl- $\lambda^5$ -C)(4,7-diphenyl-1,10-phenanthroline- $\lambda^9$ ) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 422	0.1	2
3955	3-Ethoxy-5-phenyl-1 <i>H</i> -1,2,4-triazole. IUCrData, 2019, 4, .	0.1	1
3956	( <i>R,R,S,S</i> )-9-Benzyl-3-methyl-7-phenyl-1,6-dioxo-3,9-diazaspiro[4.4]nonane-2,8-dione. IUCrData, 2019, 4, .	0.1	1
3957	6-Methyluracil: a redetermination of polymorph (II). IUCrData, 2019, 4, .	0.1	4
3958	Synthesis and crystal structure of [Cs([2.2.2]crypt)] <sub>2</sub> [Mo(CO) <sub>5</sub> ]. IUCrData, 2019, 4, .	0.1	1
3959	Benzene-1,2-diaminium bis(4-methylbenzene-1-sulfonate). IUCrData, 2020, 5, .	0.1	1
3960	2-Aminoanilinium 4-methylbenzenesulfonate. IUCrData, 2020, 5, .	0.1	2
3961	Diaquatetrakis( $\lambda^4$ -3-methoxybenzoato- $\lambda^9$ ) <sub>2</sub> $\lambda^1$ -O $\lambda^1$ -O Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 422	0.1	1
3962	Poly[ $\lambda^4$ -3,4,8,10,11,13-hexahydro-1 <i>H</i> ,6 <i>H</i> -bis([1,4]dithiocino)[6,7- <i>b</i> :6 $\epsilon^2$ ,7 $\epsilon^2$ ]pyrazine] a two-dimensional copper(I) coordination polymer. IUCrData, 2020, 5, .	0.1	1
3963	Poly[diethylammonium [tetra- $\lambda^4$ ]-cyanido- $\lambda^8$ -C: <i>N</i> -tricuprate(I)], a two-dimensional network solid. IUCrData, 2020, 5, .	0.1	1
3964	ZORKII STRUCTURAL CLASSES AND CRITICAL TOPOLOGY OF MOLECULAR CRYSTALS. Journal of Structural Chemistry, 2020, 61, 1485-1502.	0.3	9
3965	Directed Structure Formation in Tetranuclear Xylaratogermanates(IV) with Complex Phenanthrolinecopper(II) Cations. Russian Journal of Inorganic Chemistry, 2020, 65, 1703-1711.	0.3	3
3966	Inhibitory activity of metal-curcumin complexes on quorum sensing related virulence factors of <i>Pseudomonas aeruginosa</i> PAO1. AMB Express, 2020, 10, 111.	1.4	20
3967	Deflating the RNA Mg <sup>2+</sup> bubble: stereochemistry to the rescue!. Rna, 2021, 27, 243-252.	1.6	12
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4073	Crystal structure of cis-dichlorido(1,4,8,11-tetraazacyclotetradecane- $\hat{\nu}$ 4N)chromium(III) (oxalato- $\hat{\nu}$ 2O1,O2)(1,4,8,11-tetraazacyclotetradecane- $\hat{\nu}$ 4N)chromium(III) bis(perchlorate) from synchrotron data. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1417-1420.	0.2	5
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4079	Three phenanthroline $\hat{\nu}$ metal complexes with topologically similar but geometrically different conformations. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1581-1586.	0.2	0
4080	Crystal structure of N,N,N-triethylhydroxylammonium chloride. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1607-1609.	0.2	0

#	ARTICLE	IF	CITATIONS
4081	(2-Hydroxybenzoato- $\hat{\rho}$ O)triphenyl(triphenylphosphine oxide- $\hat{\rho}$ O)tin(IV). IUCrData, 2016, 1, .	0.1	0
4082	Crystal structure of 7-hydroxy-8-[(4-methylpiperazin-1-yl)methyl]-2H-chromen-2-one. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1751-1753.	0.2	1
4083	Redetermination of catena-poly[[chloridolead(II)]- $\hat{\rho}$ 42-chlorido-di- $\hat{\rho}$ 42-thiourea- $\hat{\rho}$ 4S:S] at 100 $\hat{\rho}$ ...K. IUCrData, 2016, 1, .	0.1	0
4084	(4 $\hat{\rho}$ 2-Phenyl-2,2 $\hat{\rho}$ 6 $\hat{\rho}$ 2,2 $\hat{\rho}$ 2 $\hat{\rho}$ 2-terpyridine- $\hat{\rho}$ 3N,N $\hat{\rho}$ 2,N $\hat{\rho}$ 2 $\hat{\rho}$ 2)bis(thiocyanato- $\hat{\rho}$ N)zinc(II) unknown solvate. IUCrData, 2016, 1, .		
4085	1-[(Anthracen-9-yl)carbonyl]-2,7-dimethoxynaphthalene: a chain-like structure composed of face-to-face type dimeric molecular aggregates. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1819-1823.	0.2	2
4086	Crystal structure of diethylammonium aniline-4-sulfonate anilinium-4-sulfonate. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1830-1832.	0.2	0
4087	Crystal structure of fluroxypyr. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1836-1838.	0.2	1
4088	Crystal structure of bis(bis[ $\hat{\rho}$ 3-3-methyl-3-[(4-nitro-2-oxidobenzylidene)amino]propane-1,3-diolato}tris[chlorido(dimethyl) Tj ETQq1 1,0,784314,rgBT /Over	0.2	0
4089	Crystal structure of N,N $\hat{\rho}$ 2-bis(pyridin-3-ylmethyl)cyclohexane-1,4-diammonium dichloride. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1728-1730.	0.2	0
4090	Crystal structures of two new carbazole derivatives: 12-(4-nitrophenyl)-7-phenylsulfonyl-7H-benzofuro[2,3-b]carbazole and 2-methyl-4-(4-nitrophenyl)-9-phenylsulfonyl-9H-thieno[2,3-b]carbazole. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1739-1743.	0.2	0
4091	Synthesis and structure of 1-(2-bromophenyl)-2-chloro-3-(2-chloroacetyl)-1H-indole. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 1867-1871.	0.2	0
4092	Crystal structure of {(S)-1-phenyl-N,N-bis[(pyridin-2-yl)methyl]ethanamine- $\hat{\rho}$ 3N,N $\hat{\rho}$ 2,N $\hat{\rho}$ 2 $\hat{\rho}$ 2}bis(thiocyanato- $\hat{\rho}$ N)zinc from synchrotron data. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 17-19.	0.2	1
4093	Disorder of the dimeric TCNQ $\hat{\rho}$ TCNQ unit in the crystal structure of [Ni(bpy) $\hat{\rho}$ 3 $\hat{\rho}$ 2 $\hat{\rho}$ 2(TCNQ $\hat{\rho}$ TCNQ)(TCNQ) $\hat{\rho}$ 2 $\hat{\rho}$ 2 $\hat{\rho}$ 6H $\hat{\rho}$ 2 $\hat{\rho}$ 2 O (TCNQ is) Tj ETQq0 0 0 rgBT /Overlo	0.2	1
4094	Crystal structures of two mixed-valence copper cyanide complexes with N-methylethylenediamine. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 141-146.	0.2	2
4095	Crystal structure of 1-[2-(4-chlorophenyl)-4,5-diphenyl-1 <i>H</i> -imidazol-1-yl]propan-2-ol. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 59-62.	0.2	1
4096	Crystal structures of 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(naphthalen-1-yl)acetamide and 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(4-fluorophenyl)acetamide. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 306-309.	0.2	2
4097	Vibration Spectrum Calculation Method for Solid Organic Crystals by Spectral Analysis Method. Journal of Computer Chemistry Japan, 2017, 16, 108-109.	0.0	0
4098	9-Fluoro-2,4,4a,6-tetrahydrospiro[benzo[c]chromene-3,2 $\hat{\rho}$ -[1,3]dioxolane]. IUCrData, 2017, 2, .	0.1	0



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4117	Crystal structure of 4,4-dinitro-[1,1'-biphenyl]-2-amine. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 550-552.	0.2	0
4118	Crystal structure of O-benzyl-L-tyrosine N-carboxy anhydride. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 553-555.	0.2	0
4119	Crystal structure of 2-(azaniumylmethyl)pyridinium bis(hydrogen squarate). Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 586-589.	0.2	1
4120	Crystal structure of 4-nitrophenyl 6-O-ethyl-β-D-galactopyranoside monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 598-601.	0.2	0
4122	Crystal structure of 4,5-dibromophenanthrene. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 539-542.	0.2	1
4123	3,3'-(Hexane-1,6-diyl)bis(1-vinyl-4-imidazoline-2-thione). IUCrData, 2017, 2, .	0.1	0
4124	Crystal structure and DFT study of 8-hydroxy-1,2,3,5,6,7-hexahydropyrido[3,2,1-ij]quinoline-9-carbaldehyde. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 791-794.	0.2	0
4125	Crystal structure of the 1:2 adduct of bis(piperidinium) sulfate and 1,3-dimethylthiourea. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 651-653.	0.2	0
4126	Methyl 3-(2,5-dimethoxy-3,4,6-trimethylphenyl)propanoate. IUCrData, 2017, 2, .	0.1	0
4127	5-Hydroxy-2-phenyl-7-(prop-2-yn-1-yloxy)-4H-chromen-4-one. IUCrData, 2017, 2, .	0.1	0
4128	Crystal structure of aqua-trans-bis(dimethyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 352 Td (sulfoxide- <i>l</i> O)(pyridine-2,6-dicarboxylic acid) dihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 777-779.	0.2	0
4129	The crystal structures of three pyrazine-2,5-dicarboxamides: three-dimensional supramolecular structures. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 729-734.	0.2	0
4130	Câ€”N short contacts as tools for the construction of the crystal packing in the crystal structure of 3,3'-(ethane-1,2-diyl)bis(6-iodo-3,4-dihydro-2 <i>H</i> -1,3-benzoxazine). Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 664-666.	0.2	0
4131	Crystal structure of <i>N</i> -hydroxyquinoline-2-carboxamide monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 795-797.	0.2	0
4132	Crystal structure of dibromomethoxyseselin (DBMS), a photobiologically active pyranocoumarin. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 774-776.	0.2	4
4133	The crystal structure of (C <sub>2</sub> H <sub>9</sub> N <sub>2</sub> ) <sub>2</sub> [Zn <sub>3</sub> (HPO <sub>3</sub> ) <sub>4</sub> ], a three-dimensional zincophosphite framework containing 16-membered rings templated by the unsymmetrical dimethyl hydrazinium cation. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 759-762.	0.2	2
4134	3-Hydroxy-2-phenyl-2,3,3a,7a-tetrahydro-1 <i>H</i> ,5 <i>H</i> -pyrano[3,2- <i>b</i> ]pyrrol-5-one: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 746-751.	0.2	0
4135	Crystal structure of (1 <i>Z</i> ,4 <i>Z</i> )-2,4-dimethyl-3 <i>H</i> -benzo[ <i>b</i> ][1,4]diazepine. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 647-650.	0.2	1



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4136	Crystal structures of the polymer precursors 3-(2,5-dimethoxy-3,4,6-trimethylphenyl)propyl methacrylate and 3-(2,4,5-trimethyl-3,6-dioxocyclohexa-1,4-dienyl)propyl methacrylate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 658-663.	0.2	2
4137	Different intra- and intermolecular hydrogen-bonding patterns in (3 <i>S</i> ,4 <i>S</i> ,8 <i>S</i> )-2-[(2 <i>R</i> ,3 <i>S</i> )-3-(2,5- <i>X</i> <sub>2</sub> -benzamido)-2-(2,5- <i>X</i> <sub>2</sub> -benzylamino)-2- <i>X</i> ]=H or Cl): compounds with moderate aspartyl protease inhibition activity. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 913-917.	0.2	0
4138	Crystal structure of 2-azido-1,3-bis(2,6-diisopropylphenyl)-1,3,2-diazaphospholidine. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 905-907.	0.2	2
4139	Are We Nearly There Yet?. Chemistry International, 2017, 39, 15-21.	0.3	0
4140	Crystal structure of chlorido[1-(4-nitrophenyl)thiourea- $\eta^5$ -S]bis(triphenylphosphane- $\eta^5$ -P)silver(I). Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 829-831.	0.2	1
4141	Crystal structures of three <i>N</i> -(3-acetylphenyl)quinoline-2-carboxamides. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 804-808.	0.2	0
4142	Conformational study of the 3,6-dihydro-2 <i>H</i> -1,4-oxazin-2-one fragment in 8- <i>tert</i> -butyl-7-methoxy-8-methyl-9-oxa-6-azaspiro[4.5]decane-2,10-dione stereoisomers. Acta Crystallographica Section C, Structural Chemistry, 2017, 73, 556-562.	0.2	0
4143	Crystal structure of ((1 <i>R</i> ,2 <i>R</i> )- <i>N,N</i> -bis[(quinolin-2-yl)methyl]cyclohexane-1,2-diamine)chloridoiron(III)- $\frac{1}{4}$ -oxido-[trichlorido]iron(III)chloroform monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 936-940.	0.2	1
4144	Crystal structure of ( $\alpha^+$ )-methyl (R,E)-4-[(2 <i>R</i> ,4 <i>R</i> )-2-amino-2-trichloromethyl-1,3-dioxolan-4-yl]-4-hydroxy-2-methylbut-2-enoate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 983-986.	0.2	0
4145	Crystal structure of (1 <i>E</i> ,1 <i>E</i> )-1,1-bis-(pyridine-2,6-diyl)bis[N-(2,3,4,5,6-pentafluorophenyl)ethan-1-imine]. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 954-956.	0.2	0
4146	Crystal structure of 5-[2-(9 <i>H</i> -carbazol-9-yl)ethyl]-1,3,4-oxadiazole-2(3 <i>H</i> )-thione. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1066-1069.	0.2	0
4147	Steric repulsion and supramolecular assemblies <i>via</i> a two-dimensional plate by C=H...O hydrogen bonds in two closely related 2-(benzofuran-2-yl)-2-oxoethyl benzoates. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1227-1231.	0.2	0
4148	Crystal structure of tetrahydroseselin, an angular pyranocoumarin. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1117-1120.	0.2	1
4149	Crystal structure of ethyl (E)-2-cyano-3-(thiophen-2-yl)acrylate: two conformers forming a discrete disorder. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1287-1289.	0.2	3
4150	Crystal structure and Hirshfeld surface analysis of 2-amino-4-methoxy-6-methylpyrimidinium 2-hydroxybenzoate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1305-1307.	0.2	1
4151	Crystal structure of 5-(dibenzofuran-4-yl)-2-deoxyuridine. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1493-1496.	0.2	0
4152	Crystal structure of $\beta$ -hydroxyroyleanone isolated from <i>Taxodium ascendens</i> (B.). Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1414-1416.	0.2	0
4153	Aquachlorido(2-[[6-(dimethylamino)pyrimidin-4-yl]sulfanyl]pyrimidine-4,6-diamine)copper(II) chloride hydrate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1534-1538.	0.2	0



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4154	Crystal structures of 1-benzenesulfonyl-2-methyl-3-(4-nitrobenzoyl)-2,3-dihydro-1H-indole and 1-benzenesulfonyl-2-methyl-3-[(thiophen-2-yl)carbonyl]-2,3-dihydro-1H-indole. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1555-1559.	0.2	0
4155	Supramolecular patterns and Hirshfeld surface analysis in the crystal structure of bis(2-amino-4-methoxy-6-methylpyrimidinium) isophthalate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1595-1598.	0.2	0
4156	4-Aminobenzoic acid 4-methylpyridine/4-methylpyridinium 4-aminobenzoate 0.58/0.42: a redetermination from the original data. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1508-1512.	0.2	0
4157	Crystal structure of a new polymorph of di(thiophen-3-yl) ketone. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1560-1562.	0.2	0
4158	Crystal structure of {[1- $\lambda^2$ -(diphenylphosphino)ferrocenyl]methyl}dimethylammonium chloride monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1539-1541.	0.2	0
4159	Manganese(II) chloride complexes with pyridine <i>N</i> -oxide (PNO) derivatives and their solid-state structures. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1434-1438.	0.2	5
4160	Crystal structure of 2,2- $\lambda^2$ -bipyrrole. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1517-1519.	0.2	1
4161	Crystal structure of ochraceolide A isolated from <i>Elaeodendron trichotomum</i> (Turcz.) Lundell. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1475-1478.	0.2	2
4162	A two-dimensional copper(I) coordination polymer based on 1-[2-(cyclohexylsulfanyl)ethyl]pyridin-2(1H)-one. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1782-1785.	0.2	0
4163	Crystal structure of bis( $\frac{1}{4}$ -4-bromo-2-[(2-[(2-(5-bromo-2-oxidobenzylidene)amino)ethyl]sulfanyl)sulfonyl]ethyl]imino)methyl]phenolato)dimethylformamide disolvate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1797-1800.	0.2	1
4164	Crystal structure of an epoxysterol: 9 $\beta$ ,11 $\beta$ -epoxy-5 $\alpha$ -cholest-7-ene-3 $\beta$ ,5,6 $\beta$ -triol 3,6-diacetate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1603-1606.	0.2	0
4165	The crystal structures of two isomers of 5-(phenylisothiazolyl)-1,3,4-oxathiazol-2-one. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1726-1731.	0.2	2
4166	Synthesis and crystal structure of [Pd{C <sub>6</sub> H <sub>4</sub> (CH <sub>2</sub> NHCH <sub>2</sub> Ph)-2- $\lambda^2$ - <i>N</i> ( $\frac{1}{4}$ )-solv}]} <sub>2</sub> . Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1612-1615.	0.2	0
4167	Crystal structure of (1 <i>R</i> ,5 <i>S</i> )-(endo)-(8-methyl-8-azoniabicyclo[3.2.1]oct-3-yl)ammonium aquatrifluoroborate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1712-1715.	0.2	1
4168	Crystal structure of 2,4,6-trimethylbenzoic anhydride. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1735-1738.	0.2	0
4169	Zwitterionic 1-((1 <i>E</i> )-(4-hydroxyphenyl)iminio)methyl)naphthalen-2-olate: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1674-1678.	0.2	0
4170	Crystal structure of poly[tetra- $\frac{1}{4}$ -cyanido-ethanolbis(2-iodopyrazine)digold(I)iron(II)]. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1755-1758.	0.2	1
4171	Crystal structure of {2,6-bis[(dimethylamino)methyl]phenyl- $\lambda^2$ - <i>N</i> ( $\frac{1}{3}$ )- <i>N</i> ( $\frac{1}{3}$ )- $\lambda^2$ }(bromido)chlorido)mercury(II)}. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1679-1682.	0.2	0

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4172	Crystal structure of methyl 2-[5-(2-hydroxyphenyl)-2H-tetrazol-2-yl]acetate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1971-1973.	0.2	1
4173	Crystal structure of 1,1,2-dibenzoyl-3,3,4,4-tetrakis(2-nitrophenyl)cyclobutane. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1866-1870.	0.2	0
4174	Crystal structure and Hirshfeld surface analysis of (2E,2'E)-3,3'-bis(1,4-phenylene)bis[1-(2,4-difluorophenyl)prop-2-en-1-one]. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1812-1816.	0.2	1
4175	A one-dimensional Hg(II) coordination polymer based on bis(pyridin-3-ylmethyl)sulfane. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1871-1874.	0.2	0
4176	Crystal structures of two 1:2 dihydrate compounds of chloranilic acid with 2-carboxypyridine and 2-carboxyquinoline. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1840-1844.	0.2	2
4177	Crystal structure of a zigzag Co(II) coordination polymer: catena-poly[[dichloridobis(methanol- $\kappa$ O)cobalt(II)]- $\frac{1}{4}$ -bis(pyridin-3-ylmethyl)sulfane- $\kappa^2$ N]n. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1882-1884.		
4178	Crystal structure of poly[[ $\frac{1}{4}$ -(S)-2-amino-3-hydroxypropanoato]- $\kappa$ Cis]-di- $\frac{1}{4}$ -chlorido-caesiumpalladium(II)]. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1898-1902.	0.2	0
4179	Crystal structure of a diaryl carbonate: 1,3-phenylene bis(phenyl carbonate). Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1942-1945.	0.2	0
4180	Crystal structure of 3,6,6-trimethyl-4-oxo-1-(pyridin-2-yl)-4,5,6,7-tetrahydro-1H-indazol-7-aminium chloride and its monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1931-1936.	0.2	0
4181	Crystal structure of (1S,4S)-2,5-diazoniabicyclo[2.2.1]heptane dibromide. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1861-1865.	0.2	3
4182	Crystal structure of (1S,2R)-2-hydroxy-1,2-diphenylethan-1-aminium (S)-2-azaniumylbutanedioate monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1827-1830.	0.2	0
4183	Nitrosonium complexation by the tetrakisphosphonate cavitand 5,11,17,23-tetramethyl-6,10:12,16:18,22:24,4-tetrakis(phenylphosphonato- $\kappa^2$ O, $\kappa^2$ O)resorcin(4)arene. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1801-1805.		
4184	Sustaining Scholarly Infrastructures through Collective Action: The Lessons that Olson can Teach us. KULA Knowledge Creation Dissemination and Preservation Studies, 0, 1, 3.	0.3	5
4185	Crystal structure of 6,7-dehydroroyleanone isolated from <i>Taxodium distichum</i> (L.) Rich.. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 62-64.	0.2	1
4186	Crystal structure of 3-[(2-acetamidophenyl)imino]butan-2-one. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 193-195.	0.2	0
4187	Hydrogen Bond Contribution to Drug Bioavailability: cheminformatics approach. Biomedical Chemistry Research and Methods, 2018, 1, e00060.	0.1	1
4188	DIRECT SYNTHESIS AND CRYSTAL STRUCTURE OF BIS(BROMIDO-BIS(1,10-PHENANTHROLINE)-COPPER(II)) NITROPRUSSIDE DIMETHYLFORMAMIDE SOLVATE. Bulletin of Taras Shevchenko National University of Kyiv Chemistry, 2018, , 15-18.	0.1	0
4189	Crystal structures of bis[4-(dimethylamino)pyridinium] tetrakis(thiocyanato- $\kappa^2$ N)manganate(II) and tris[4-(dimethylamino)pyridinium] pentakis(thiocyanato- $\kappa^2$ N)manganate(II). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 15-20.	0.2	1



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4208	Effect of counter-ion on packing and crystal density of 5,5â€²-(3,3â€²-bi[1,2,4-oxadiazole]-5,5â€²-diy)bis(1<i>H</i>-tetrazol-1-olate) with five different cations. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 505-513.	0.2	2
4209	Crystal structure of (20<i>S</i>)-21-[4-(2-hydroxypropan-2-yl)-1<i>H</i>-1,2,3-triazol-4-yl]-20-(4-methylpentyl)-5-pregnen-3â€²-ol with an unknown solvate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 465-468.	0.2	1
4210	Crystal structure of <i>catena</i>-poly[[diiodidomercury(II)]-â€²/4-2,2â€²-dithiobis(pyridine)] Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 667 Td Communications, 2018, 74, 433-435.	0.2	2
4211	Crystal structure of [2,13-bis(acetamido)-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.0<sup>7,12</sup>]docosane-â€²<sup>4</sup><i>N</i>]silver(II) dinitrate from synchrotron X-ray data. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 461-464.	0.2	1
4212	Crystal structure of 2,3-bis(4-methylphenyl)benzo[<i>g</i>]quinoxaline. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 548-550.	0.2	0
4213	Crystal structure of bis(diisopropylammonium) <i>cis</i>-diiodidobis(oxolato-â€²<sup>2</sup><i>O</i>) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 667 Td Communications, 2018, 74, 502-504.	0.2	2
4214	Crystal structure of 2-[[[8-aminonaphthalen-1-yl)imino]methyl]-4,6-di-<i>tert</i>-butylphenolato-â€²<sup>3</sup>) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 500 Communications, 2018, 74, 469-473.	0.2	0
4215	Crystal structure of 5-[2-(2,4,6-tribromophenyl)diazenyl]tropolone. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 709-712.	0.2	0
4216	Crystal structure of strontium and barium acesulfame (6-methyl-4-oxo-4H-1,2,3-oxathiazin-3-ide) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 667 Td Communications, 2018, 74, 433-435.	0.2	1
4217	Crystal structure and Hirshfeld surface analysis of 2-oxo-13-epi-manoyl oxide isolated from <i>Sideritis perfoliata</i>. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 713-717.	0.2	1
4218	Crystal structures and Hirshfeld surface analyses of 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-<i>N</i>-[(pyridin-2-yl)acetamide and 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-<i>N</i>-[(pyrazin-2-yl)acetamide. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 718-723.	0.2	0
4219	Expected and unexpected products of reactions of 2-hydrazinylbenzothiazole with 3-nitrobenzenesulfonyl chloride in different solvents. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 673-677.	0.2	2
4220	Crystal structure of difluorido{2-[(4-hydroxyphenyl)diazenyl]-3,5-dimethylpyrrolido}boron. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 743-746.	0.2	0
4221	Crystal structure of 2-{5-[2-(2-hydroxyphenyl)diazen-1-yl]-1-methylpyrrol-2-yl}phenol methanol monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 871-873.	0.2	0
4222	A rare positively charged nicotinic acid disulfide: 2,2â€²-dithiodinicotinic acid hydrochloride monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 820-824.	0.2	0
4223	Synthesis, spectroscopic and Hirshfeld surface analysis and fluorescence studies of (2<i>E</i>)-2â€²<i>E</i>-3,3â€²-(1,4-phenylene)bis[1-(4-hydroxyphenyl)prop-2-en-1-one] <i>N</i>-<i>N</i>-dimethylformamide disolvate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 835-839.	0.2	0
4224	Crystal structure of (â€²)-(<i>R</i>,<i>E</i>)-3-(1,3-benzodioxol-5-yl)-5-[(4<i>S</i>,5<i>R</i>)-5-hydroxymethyl-2,2-dimethyl-1,3-dioxolane-4-yl]-<i>N</i>-<i>N</i>-dimethylformamide disolvate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 825-828.	0.2	0
4225	Crystal structures of binary compounds of meldonium 3-(1,1,1-trimethylhydrazin-1-ium-2-yl)propanoate with sodium bromide and sodium iodide. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 829-834.	0.2	1

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4226	Crystal structure of 1-[3,5-bis(trifluoromethyl)phenyl]-2-bromoethan-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 868-870.	0.2	0
4227	Crystal structure of a heterometallic coordination polymer: <i>catena</i> -poly[[[tetraaquacobalt(II)]-1/4-pyridine-2,6-dicarboxylato-calcium(II)-1/4-pyridine-2,6-dicarboxylato] dihydrate]. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 808-811.	0.2	1
4228	Sodium rubidium disaccharinate tetrahydrate. IUCrData, 2018, 3, .	0.1	0
4229	Crystal structure of the tetramethyl(phenethyl)cyclopentadienylmolybdenumtricarbonyl dimer. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1017-1020.	0.2	0
4230	Crystal structure of <i>N</i> -[1-(4-aminophenyl)ethylidene]-2-hydroxy-5-iodobenzohydrazide methanol monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 910-914.	0.2	1
4231	Crystal structure and theoretical study of (2 <i>E</i> )-1-[4-hydroxy-3-(morpholin-4-ylmethyl)phenyl]-3-(thiophen-2-yl)prop-2-en-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 960-963.	0.2	2
4232	Crystal structure of (2,2'-bipyridine) <sup>2+</sup> Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 507 Td ( <i>N</i> , <i>N</i> )- <i>trans</i> - <i>N,N'</i> - Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 970-972.	0.2	0
4233	Crystal structures of sodium-, lithium-, and ammonium 4,5-dihydroxybenzene-1,3-disulfonate (tiron) hydrates. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 918-925.	0.2	0
4234	Crystal structure of 2-[2-(pyridin-3-yl)diazen-1-yl]aniline. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1013-1016.	0.2	0
4235	Crystal structure of ( <i>E</i> )-2-( <i>tert</i> -butylamino)-4-( <i>tert</i> -butylimino)naphthalen-1(4 <i>H</i> )-one. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 973-976.	0.2	1
4236	Crystal structure of tris[(pyridin-1-ium-2-yl)methyl]amine trichloride·methanol·water (1/1.829/0.342). IUCrData, 2018, 3, .	0.1	0
4237	{N 1-[2-(Butylselanyl)benzyl]-N 2,N 2-dimethylethane-1,2-diamine}dichloridomercury(II). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1151-1154.	0.2	0
4238	(2 <i>R</i> ,3 <i>R</i> )-1,4-Dioxaspiro[4.4]nonane-2,3-dicarboxylic and (2 <i>R</i> ,3 <i>R</i> )-1,4-dioxaspiro[4.5]decane-2,3-dicarboxylic acids. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1058-1062.	0.2	0
4239	5,5-Diphenyl-2-thioxoimidazolidin-4-one dimethyl sulfoxide monosolvate. IUCrData, 2018, 3, .	0.1	4
4240	Crystal structure of tetrakis(1,1,1,5,5,5-hexafluoroacetylacetonato)hafnium(IV). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1182-1185.	0.2	0
4241	Crystal structures of 2-bromo-1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilane and 2-bromo-1,1,1,3,3,3-hexaisopropyl-2-(triisopropylsilyl)trisilane. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1142-1146.	0.2	0
4242	Crystal structures of $\text{Zn}^{\text{II}}\text{Gly}^{\text{I}}\text{Aib}^{\text{I}}\text{O}^{\text{II}}\cdot 0.5\text{Ca}^{2+}\cdot \text{H}_2\text{O}$ and $\text{Zn}^{\text{II}}\text{Gly}^{\text{I}}\text{Aib}^{\text{I}}\text{OH}$ . Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1173-1177.	0.2	0
4243	Crystal structure of aqua(2-[[2-([2-bis(carboxylato- <sup>18</sup> O-methyl)amino- <sup>15</sup> N]ethyl)(carboxylato- <sup>18</sup> O-methyl)amino- <sup>15</sup> N]ethyl)(carboxymethyl)azaniumyl]acetato) trihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1054-1057.		



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4244	Crystal structure and Hirshfeld surface analysis of ethyl (E)-4-[(4-hydroxy-3-methoxy-5-nitrobenzylidene)amino]benzoate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1079-1082.	0.2	0
4245	Crystal structures of dimethyl 5-iodoisophthalate and dimethyl 5-ethynylisophthalate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1093-1096.	0.2	0
4246	Tris(4-methoxyphenyl)stibine. IUCrData, 2018, 3, .	0.1	0
4247	Crystal structure and redox potentials of the tppz-bridged {RuCl(bpy)} <sub>2</sub> dimer. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1250-1253.	0.2	0
4248	Bis(3-carbamoylpyridin-1-ium) phosphite monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1295-1298.	0.2	0
4249	Crystal structure of 3-(triphenylphosphoranylidene)-2,5-dihydrofuran-2,5-dione tetrahydrofuran monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1336-1338.	0.2	0
4250	Structures of the diiodine adducts of bis(diisopropylphosphano)methane disulfide and bis(diisopropylphosphano)ethane disulfide. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2018, 73, 669-672.	0.3	0
4251	Crystal structure of (S)-1-O-tert-butylidiphenylsilylglycerol: eight chiral molecules in a triclinic cell. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1373-1379.	0.2	0
4252	Crystal structure and Hirshfeld surface analysis of methyl 4-[(E)-2-(5-bromo-2-methoxybenzylidene)hydrazinyl]-3-nitrobenzoate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1239-1243.	0.2	0
4253	Crystal structure of fac-bis[bis(pyridin-2-yl)methanamine]iron(II) 1,1,3,3-tetracyano-2-(dicyanomethylidene)propane-1,3-diide, [Fe(dipa) <sub>2</sub> ](tcpd). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1227-1230.	0.2	1
4254	Crystal structure of bis(pivaloylhydroxamato- $\eta^2$ O,O $\eta^2$ )copper(II). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1384-1387.	0.2	0
4255	Crystal structures of the hexafluoridophosphate salts of the isomeric 2-, 3- and 4-cyano-1-methylpyridinium cations and determination of solid-state interaction energies. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1322-1329.	0.2	0
4256	Crystal structure of $[\text{C}_{10}\text{H}_{12}\text{N}_2\text{C}_2\text{O}_2]^{2+}$ 4:2(1,2,3,4- $\lambda^1$ )-1,2,3,4-tetraphenylbuta-1,3-diene-1,4-diyl]bis(tricarbonyl-osmium)(Os $\eta^5$ -Os). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1235-1238.	0.2	0
4257	Crystal structure determination of $(\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}_2)^{2+}$ (1-acetyl-1H-indazol-3-yl)-1H-imidazole-2,1,17-dihydro-10H-spiro[indene-2,18 $\eta^5$ -5a]acetone 1.5-solvate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1444-1447.	0.2	0
4258	Template or ligand? Different structural behaviours of aromatic amines in combination with zincophosphite networks. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1411-1416.	0.2	2
4259	Ethyl 6-cyano-7-phenyl-6,7-tetrahydro-3H-spiro[indeno[1,2-b]quinoxaline-11,5 $\eta^5$ pyrrolo[1,2-c]pyridine]octane. IUCrData, 2018, 3, .		
4260	Bis[(4-chlorophenoxy)acetato- $\eta^3$ O<math>/i>](ethylenediamine- $\eta^2$ N<math>/i>, <math>/i>N<math>/i> $\eta^2$ )zinc. IUCrData, 2018, 3, .	0.1	2
4261	Pyridine-3-carboxamide $\eta^2$ telluric acid (1/1). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1521-1525.	0.2	0



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4262	Crystal structure and Hirshfeld surface analysis of diethyl 2-[4-(4-fluorophenyl)-2-methyl-4-oxobutan-2-yl]malonate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1388-1391.	0.2	0
4263	Crystal structure of ( $\eta^5$ -cyclooctadiene)(3,3-dimesityl-1,1-methylenediimidazole-2,2-diyldiene)nickel(0) tetrahydrofuran monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1396-1399.	0.2	2
4264	Crystal Structure of ( <i>E</i> )-2-(3,3,3-trifluoroprop-1-en-1-yl)aniline. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1448-1450.	0.2	0
4265	Crystal structures of the solvent-free and ethanol disolvate forms of 4,4-diazenediylbis(2,3,5,6-tetrafluorobenzoic acid) exemplifying self-stabilized azobenzene <i>cis</i> -configurations. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1486-1490.	0.2	0
4266	Different classical hydrogen-bonding patterns in three salicylaldoxime derivatives, 2-HO-4-X-C <sub>6</sub> H <sub>3</sub> C=NOH (X = Me, OH and MeO). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1480-1485.	0.2	1
4267	Crystal structure of ( <i>E</i> )-2-[3-( <i>tert</i> -butyl)-2-hydroxybenzylidene]- <i>N</i> -cyclohexylhydrazine-1-carbothioamide. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1460-1462.	0.2	3
4268	[Bis(2,6-diisopropylphenyl) phosphato- $\eta^5$ O]pentakis(methanol- $\eta^5$ O)manganese bis(2,6-diisopropylphenyl) phosphate methanol trisolvate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1433-1438.	0.2	1
4269	Investigation of nitro-nitrito photoisomerization: crystal structures of <i>trans</i> -bis(acetylacetonato- $\eta^5$ O, $\eta^5$ O)(pyridine/4-methylpyridine/3-hydroxypyridine)nitrocobalt(III). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1637-1642.	0.2	3
4270	Crystal structure of bis(diisopropylammonium) molybdate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1682-1685.	0.2	2
4271	Crystal structure of bis[( <i>S</i> )-2-(2-hydroxybenzylamino)-4-methylpentanoato- $\eta^2$ <i>N</i> , $\eta^5$ O] (1,10-phenanthroline- $\eta^2$ <i>N</i> , $\eta^5$ O)cadmium dihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1565-1568.	0.2	1
4272	The first spontaneous resolution of a sulfoxide: Dianin's compound analogue, ( <i>R</i> )-4-(4-hydroxyphenyl)-2,2,4-trimethylthiachroman-1-oxide. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1633-1636.	0.2	0
4273	Crystal structure and Hirshfeld analysis of 2-[bis(1-methyl-1 <i>H</i> -indol-3-yl)methyl]benzoic acid. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1580-1583.	0.2	0
4274	Crystal structure and Hirshfeld surface analysis of ( <i>Z</i> )-4-chloro- $\eta^2$ -(4-oxothiazolidin-2-ylidene)benzenesulfonohydrazide monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1569-1573.	0.2	0
4275	Crystal structure at 100 K of bis[1,2-bis(diphenylphosphanyl)ethane]nickel(II) bis(trifluoromethanesulfonate): a possible negative thermal expansion molecular material. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1678-1681.	0.2	0
4276	The solid-state conformation of the topical antifungal agent <i>O</i> -naphthalen-2-yl <i>N</i> -methyl- <i>N</i> -(3-methylphenyl)carbamothioate. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 1495-1501.	0.2	2
4277	Crystal structure of 1-butyl-3-{2-[(indan-5-yl)amino]-2-oxoethyl}-1 <i>H</i> -imidazol-3-ium chloride. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1665-1668.	0.2	0
4278	Crystal structure of 13-( <i>E</i> )-(2-aminobenzylidene)parthenolide. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1543-1546.	0.2	0
4279	Crystal structure of <i>N</i> -isopropyl- <i>N</i> -(phenyl)phenylglyoxylamide. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1574-1576.	0.2	0

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4280	Crystal structure and Hirshfeld surface analysis of dimethyl (3 <i>a</i> - <i>S</i> ,6 <i>a</i> - <i>R</i> ,6 <i>a</i> - <i>S</i> ,7 <i>a</i> - <i>S</i> )-2-(2,2,2-trifluoroacetyl)-2,3-dihydro-1 <i>H</i> ,6 <i>H</i> ,7 <i>H</i> -3 <i>a</i> ,6 <i>a</i> ,7,9-diaepoxybenzo Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1599-1604.	0.2	0
4281	Crystal structure and optical spectroscopic analyses of (<i>E</i>)-3-(1<i>H</i>-indol-2-yl)-1-(4-nitrophenyl)prop-2-en-1-one hemihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1589-1594.	0.2	4
4282	Crystal structure of dichloridobis{[1/4-2-methoxy-6-[(methylimino)methyl]phenolato}{2-methoxy-6-[(methylimino)methyl]phenolato}cadmium(II)cobalt(III) monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1532-1535.	0.2	0
4283	The methanol sesquisolvate of sodium naproxen. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1624-1627.	0.2	1
4284	Crystal structures and Hirshfeld surfaces of four methoxybenzaldehyde oxime derivatives, 2-MeO-<i>X</i><sub>6</sub><sub>H</sub><sub>3</sub><sub>C</sub>=NOH (<i>X</i>= H and 2-, 3- and 4-MeO): different conformations and hydrogen-bonding patterns. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1553-1560.	0.2	0
4285	Crystal structure and Hirshfeld surface analysis of tetraaquis(isonicotinamide- $\hat{N}$ ) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T 2018, 74, 1536-1539.	0.2	1
4286	Structure of 2-chloro-<i>N</i>-(<i>p</i>-tolyl)propanamide. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1584-1588.	0.2	2
4287	Charge-assisted hydrogen bonding in three diaminobenzene salts. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 1725-1731.	0.2	2
4288	Structures of the hydrate and dihydrate forms of the DNA-binding radioprotector methylproamine. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1903-1907.	0.2	0
4289	Crystal structures of two stilbazole derivatives: bis{(<i>E</i>)-4-[4-(diethylamino)styryl]-1-methylpyridin-1-ium} tetraiodidocadmium(II) and (<i>E</i>)-4-[4-(diethylamino)styryl]-1-methylpyridin-1-ium 4-methoxybenzenesulfonate monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1891-1894.	0.2	0
4290	Polymorphism in some new bis-hydrazone compounds. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 1656-1666.	0.2	2
4291	The enrichment ratio of atomic contacts in the crystal structure of isomeric, triply protonated, 4 $\hat{E}^2$ -functionalized terpyridine cations with [ZnCl<sub>4</sub>] <sup>2+</sup> as counter-ion. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1881-1886.	0.2	0
4292	Crystal structure of di- $\hat{1}/4$ -hydroxido-bis{aqua[ethyl (1,10-phenanthrolin-3-yl)phosphonato- $\hat{P}$ <sup>2</sup>]} copper(II)} heptahydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1751-1754.	0.2	0
4293	Synthesis, molecular structure and Hirshfeld surface analysis of (4-methoxyphenyl)[2-(methylsulfanyl)thiophen-3-yl]methanone. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1800-1803.	0.2	0
4294	Investigation of nitro $\hat{E}$ -nitrito photoisomerization: crystal structure of<i>trans</i>-chloridonitro(1,4,8,11-tetraazacyclotetradecane- $\hat{P}$ <sup>4</sup>)<i>N</i>, <i>N</i>- $\hat{E}^2$ , <i>N</i>- $\hat{E}^2$ and <i>N</i>- $\hat{E}^2$ chloride. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1908-1912.	0.2	0
4295	Chemo- and regioselective [3 $\hat{A}+2$ ]-cycloadditions of thiocarbonyl ylides: crystal structures of <i>trans</i>-8-benzoyl-1,1,3,3-tetramethyl-7-trifluoromethyl-5-thiaspiro[3.4]octan-2-one and <i>trans</i>-3-benzoyl-2,2-diphenyl-4-(trifluoromethyl)tetrahydrothiophene. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1705-1709.	0.2	0
4296	Packing polymorphism in the structure of<i>trans</i>-aqua<i>N</i>, <i>N</i>- $\hat{E}^2$ -bis(salicylidene)ethane-1,2-diamine- $\hat{P}$ <sup>4</sup> <i>O</i>, <i>N</i>, <i>O</i>- $\hat{E}^2$ <i>O</i>- $\hat{E}^2$ monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1778-1782.	0.2	0
4297	Tetrakis(4-benzoylpyridine- $\hat{P}$ <i>N</i>)-bis(isothiocyanato- $\hat{P}$ <i>N</i>)-manganese(II). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1899-1902.	0.2	3

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4298	Two polymorphic forms of the oxathiin systemic fungicide active carboxine. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1741-1745.	0.2	1
4299	Synthesis and crystal structures of 5,5-dimethyl-(propane-2,2-diyl)bis(2-hydroxybenzaldehyde) and 5,5-dimethyl-(propane-2,2-diyl)bis(2-hydroxyisophthalaldehyde). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1872-1877.	0.2	0
4300	Crystal structure of poly[bis(1/4-2-bromopyrazine)tetra-1/4<sub>2</sub>-cyanido-dicopper(I)iron(II)]: a bimetallic metal-organic framework. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1895-1898.	0.2	1
4301	Structures and phase transition of three isomers of 1-phenylindolin-2-one derivatives: 6-chloro-1-phenylindolin-2-one, 4-chloro-1-phenylindolin-2-one and 1-(3-chlorophenyl)indolin-2-one. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 1750-1758.	0.2	0
4302	Formation and structural characterization of a potassium amidinoguanidinate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1795-1799.	0.2	0
4303	(1/4-Methylenediphosphonato) <sup>2-</sup> Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 547 Td (<i>O</i>,<i>O</i>)<sup>2</sup>-<i>O</i> tetrahydrate. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1838-1841.	0.2	0
4304	Investigation of nitro-nitrito photoisomerization: crystal structures of <i>trans</i>-{2,2-bis[ethane-1,2-diylbis(nitrimethylidene)]diphenolato}(pyridine/4-methylpyridine)nitrocobalt(III). Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1759-1763.	0.2	2
4305	Crystal structure of bis(1/4<sub>2</sub>-methanolato) <sup>2-</sup> hexamethylbis(1/4<sub>2</sub>-triphenylacetato) <sup>2-</sup> . Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1790-1794.	0.2	0
4306	2-[2,8-Bis(trifluoromethyl)quinolin-4-yl](hydroxy)methylpiperidin-1-ium trichloroacetate: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1851-1856.	0.2	3
4307	A 1:2 co-crystal of 2,2-thiodibenzoic acid and triphenylphosphane oxide: crystal structure, Hirshfeld surface analysis and computational study. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1764-1771.	0.2	9
4308	Hydrogen-bonding chain and dimer motifs in pyridinium and morpholinium hydrogen oxalate salts. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1804-1807.	0.2	1
4309	Crystal structure of the ethyl 2,4-dihydroxy-6-methylbenzoate from <i>Illicium difengpi</i> K.I.B et K.I.M.. IUCrData, 2018, 3, .	0.1	0
4311	(<i>Z</i>)-3-Butyl-5-(4-nitrobenzylidene)thiazolidine-2,4-dione. IUCrData, 2019, 4, .	0.1	0
4312	Crystal structure determination of two pyridine derivatives: 4-[(<i>E</i>)-2-(4-methoxyphenyl)ethenyl]-1-methylpyridin-1-ium hexafluoro- <sup>6-</sup> -phosphane and 4-[(<i>E</i>)-2-[4-(dimethylamino)phenyl]ethenyl]-1-phenyl- <sup>5-</sup> -pyridin-1-ylum hexafluoro- <sup>6-</sup> -phosphane. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 288-291.	0.2	0
4313	Crystal structure, Hirshfeld surface analysis and electrostatic potential study of naturally occurring cassane-type diterpenoid Pulcherrimin C monohydrate at 100 K. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 119-123.	0.2	0
4314	Dichlorido(2,2-methylenedipyridine)zinc(II). IUCrData, 2019, 4, .	0.1	0
4315	Synthesis, molecular and crystal structure of 1-(1,2-dihydrophthalazin-1-ylidene)-2-[1-(thiophen-2-yl)ethylidene]hydrazine. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 251-254.	0.2	7
4316	Crystal structure and Hirshfeld surface analysis of a bromochalcone: (<i>E</i>)-1-(3-bromophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 264-267.	0.2	1

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4317	Synthesis, characterization and crystal structure determination of new coordination polymers of cadmium (II) based on pyridine hydrazide ligands. Iranian Journal of Crystallography and Mineralogy, 2019, 26, 1001-1012.	0.0	2
4318	Crystal structure of the co-crystal salt 2-amino-6-bromopyridinium 2,3,5,6-tetrafluorobenzoate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 284-287.	0.2	0
4319	A new, deep quinoxaline-based cavitand receptor for the complexation of benzene. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 103-108.	0.2	0
4320	Crystal structure of (1,3-thiazole-2-carboxylato- $\lambda^5$ -(1,3-thiazole-2-carboxylic) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 62 185-188.	0.2	4
4321	Crystal structure and Hirshfeld surface analysis of poly[[di- $\frac{1}{4}$ -sub>3</sub>-glycine-lithium] perchlorate]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 134-138.	0.2	1
4322	Crystal structure of 3,6-bis(pyridin-2-yl)-1,4-dihydro-1,2,4,5-tetrazine. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 86-88.	0.2	0
4323	Hydrogen-bonded molecular salts of reduced benzothiazole derivatives with carboxylates: a robust R <sub>2</sub> <sup>2</sup> (8) supramolecular motif (even when disordered). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 167-174.	0.2	1
4324	Crystal structures of 2,3-bis(thiophen-2-yl)pyrido[2,3- <i>b</i> ]pyrazine and 7-bromo-2,3-bis(thiophen-2-yl)pyrido[2,3- <i>b</i> ]pyrazine. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 89-93.	0.2	0
4325	Crystal structure of <i>trans</i> -bis[2-(1- <i>H</i> -benzotriazol-1-yl)acetato- $\lambda^5$ -O]bis(ethanolamine- $\lambda^2$ ) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 62 75, 233-236.	0.2	0
4326	Crystal structure of ( <i>trans</i> )-4-(3-carboxy-1-ethyl-6,8-difluoro-4-oxo-1,4-dihydroquinolin-7-yl)-2-methylpiperazin-1-ium 3-carboxy-5-fluorobenzoate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 68-70.	0.2	0
4327	Crystal structures of 6a,6b,7,11a-tetrahydro-6- <i>H</i> ,9- <i>H</i> -spiro[chromeno[3,4- <i>b</i> ]pyrrolo[1,2- <i>c</i> ]thiazole-11,3-indoline]-2,6-dione and 5a,5b,6,7,11a-tetrahydro-6- <i>H</i> ,9- <i>H</i> -spiro[chromeno[3,4- <i>b</i> ]pyrrolo[1,2- <i>c</i> ]thiazole-11,3-indoline]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 246-250.	0.2	0
4328	Crystal structure and Hirshfeld surface analysis of 5-[(5-nitro-1- <i>H</i> -indazol-1-yl)methyl]-3-phenyl-4,5-dihydroisoxazole. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 71-74.	0.2	3
4330	Conformational dimorphism of 2,2-methylenebis(isoindoline-1,3-dione). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 49-52.	0.2	0
4331	Crystal structure of 6-(4-chlorophenyl)-6a-nitro-6a,6b,8,9,10,12a-hexahydro-6- <i>H</i> ,7- <i>H</i> -spiro[chromeno[3,4- <i>a</i> ]indolizine-12,11-indole]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 255-259.	0.2	0
4332	The crystal structures of 6-(4-chlorophenyl)- and 6-(4-methoxyphenyl)-6a-nitro-6a,6b,8,9,10,12a-hexahydro-2- <i>H</i> ,6- <i>H</i> ,8- <i>H</i> -spiro[acetylacetonate-10,11-indole]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 218-222.	0.2	0
4333	Crystal structure of 7a-(4-chlorophenyl)-2a-(4-methoxyphenyl)-7a',7a''-tetrahydro-1- <i>H</i> ,3- <i>H</i> ,5- <i>H</i> and an unknown solvent. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 189-193.	0.2	0
4334	Crystal structure of a host-guest complex between mephedrone hydrochloride and a tetraphosphonate cavitand. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 277-283.	0.2	0
4335	Crystal structure of benzyl 2-naphthyl ether, a sensitiser for thermal paper. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 242-245.	0.2	2

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4336	Crystal structure of 4-[(adamantan-1-yl)amino]naphthalene-1,2-dione. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 99-102.	0.2	0
4337	Crystal structure and Hirshfeld surface analysis of $\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}_2$ -[ethane-1,2-diylbis(oxy)]bis(4-methylbenzenesulfonamide). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 81-85.	0.2	1
4338	Crystal structure of bis(4-benzoylpyridine- $\eta^5$ -C <sub>5</sub> H <sub>4</sub> N) $\eta^2$ -O-bis(thiocyanato- $\eta^1$ -C <sub>4</sub> H <sub>3</sub> N)nickel(II) methanol monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 299-303.	0.2	2
4339	Crystal structure of 2-[(2E)-2-methyl-3-phenylprop-2-en-1-ylidene]-N-phenylhydrazinocarboxamide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 163-166.	0.2	1
4340	Crystal structure and Hirshfeld surfaces analysis of the nickel(II) complex of the Schiff base ligand 6,6'-bis[2-(trifluoromethoxy)phenyl]-[ethane-1,2-diylbis(azanylylidene)]bis(methanylylidene)phenol]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 328-331.	0.2	1
4341	Crystal structure of idelalisib tert-butanol monosolvate dihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 414-417.	0.2	0
4342	Crystal structure, Hirshfeld surface analysis and frontier molecular orbital analysis of (E)-4-bromo-N-(2,3-dichlorobenzylidene)benzohydrazide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 324-327.	0.2	1
4343	Crystal structure, Hirshfeld surface analysis and DFT study of (2Z)-2-(4-fluorobenzylidene)-4-(prop-2-yn-1-yl)-3,4-dihydro-2H-1,4-benzothiazin-3-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 372-377.	0.2	6
4344	Crystal structure of chlorido{tris[2-(isopropylsulfanyl)phenyl]phosphane- $\eta^3$ -4C <sup>+</sup> }nickel(II) trifluoromethanesulfonate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 350-353.	0.2	0
4345	Crystal structures of two nickel(II) macrocyclic salts: (5,7,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane)nickel(II) bis(perchlorate) monohydrate and (5,7,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane)nickel(II) dibromide trihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 332-337.	0.2	0
4346	Crystal structure and magnetic properties of (tris{4-[1-(2-methoxyethyl)imidazol-2-yl]-3-azabut-3-enyl}amine)iron(II) bis(hexafluoridophosphate). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 358-361.	0.2	1
4347	Crystal structure of a host-guest complex of the tris-urea receptor, 3-(4-nitrophenyl)-1,1-bis[2-[3-(4-nitrophenyl)ureido]ethyl]urea, that encapsulates hydrogen-bonded chains of dihydrogen phosphate anions with separate tetra-n-butylammonium counter-ions. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 319-323.	0.2	0
4348	Diethyl 3,3'-bis[(4-fluorophenyl)methylidene]bis(1H-indole-2-carboxylate). IUCrData, 2019, 4, .	0.1	0
4349	Crystal structure and Hirshfeld surface analysis of two 5,11-methanobenzo[ <i>g</i> ][1,2,4]triazolo[1,5- <i>c</i> ][1,3,5]oxadiazocine derivatives. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 492-498.	0.2	2
4350	Crystal structure and Hirshfeld surface analysis of 2-(1H-indol-3-yl)ethanaminium acetate hemihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 451-455.	0.2	1
4351	Crystal structure and Hirshfeld surface analysis of dimethyl (1R,3aS,3a <sup>+</sup> )Tj ETQq1 1 0.784314 rgBT /Overl. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 460-464.	0.2	0
4352	Quantitative analysis of weak non-covalent interactions in (Z)-3-(4-chlorophenyl)-2-phenylacrylonitrile: insights from PIXEL and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 499-505.	0.2	1
4353	(E)-3-Methyl-2,5-bis(4-methylbenzylidene)cyclopentanone: synthesis, characterization, Hirshfeld surface analysis and antibacterial activity. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 506-511.	0.2	0



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4354	A 1:1:1 co-crystal solvate comprising 2,2-dithiodibenzoic acid, 2-chlorobenzoic acid and <i>N,N</i> -dimethylformamide: crystal structure, Hirshfeld surface analysis and computational study. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 475-481.	0.2	3
4355	Crystallographic and spectroscopic characterization of 4-nitro-2-(trifluoromethyl)benzoic acid and 4-nitro-3-(trifluoromethyl)benzoic acid. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 524-528.	0.2	1
4356	Crystal structure of bis( $\eta^2$ -triphenylacetato- $\eta^1$ -O) $\eta^2$ bis(diisobutylaluminium). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 456-459.	0.2	0
4357	The crystal structures of two new coumarin derivatives: 2-(4-{2-[(2-oxo-2H-chromen-4-yl)oxy]acetyl}piperazin-1-yl)acetamide and <i>N,N</i> -(2,4-dimethoxybenzyl)-2-[(2-oxo-2H-chromen-4-yl)oxy]acetamide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 482-488.	0.2	1
4358	Crystal structure of bis[bis(1,4,7-triazacyclononane- $\eta^3$ )chromium(III)] tris(tetrachloridozincate) monohydrate from synchrotron X-ray data. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 428-431.	0.2	1
4359	( <i>Z</i> )-3-([3-Methoxy-5-(trifluoromethyl)phenyl]imino)methyl)benzene-1,2-diol. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 470-474.	0.2	3
4360	Crystal structure of bis( $\eta^2$ -2-methoxy-6-[(methylimino)methyl]phenolato)bis({2-methoxy-6-[(methylimino)methyl]phenolato}nickel(II)) involving different coordination modes of the same Schiff base ligand. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 620-623.	0.2	1
4361	Bis(3-methylsalicylato)bis(picolinamide)copper(II) complex $\alpha^{\text{II}}$ preparation, spectral properties and supposed structure. <i>Acta Chimica Slovaca</i> , 2019, 12, 97-102.	0.5	0
4362	Crystal structure of <i>trans</i> -diaqua(3,10-dimethyl-1,3,5,8,10,12-hexaazacyclotetradecane)copper(II) pamoate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 533-536.	0.2	1
4363	Crystal structure, Hirshfeld surface analysis and DFT study of (2- <i>Z</i> )-2-(2,4-dichlorobenzylidene)-4-[2-(2-oxo-1,3-oxazolidin-3-yl)ethyl]-3,4-dihydro-2H-1,4-benzothiazin-3-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 593-599.	0.2	6
4364	( <i>E</i> )-2-(2-Hydroxy-3-methylbenzylidene)- <i>N,N</i> -methylhydrazine-1-carbothioamide: supramolecular assemblies in two-dimensions mediated by $\text{N}\cdots\text{H}\cdots\text{S}$ and $\text{C}\cdots\text{H}\cdots\text{N}$ interactions. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 571-575.	0.2	0
4365	Crystal structure and Hirshfeld surface analysis of ( <i>E</i> )-2-[1-hydroxy-2-(pyridin-2-yl)ethyl]-4-[2-(4-methoxyphenyl)diazene-1-yl]phenol. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 600-603.	0.2	0
4366	Crystal structure of <i>fac</i> -aqua[( <i>E</i> )-4-(benzo[ <i>d</i> ]thiazol-2-yl)- <i>N,N</i> -(pyridin-2-ylmethylidene)aniline- $\eta^2$ )tricarbonylrhenium(I) hexafluoridophosphate methanol monosolvate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 580-584.	0.2	0
4367	Crystal structure of 1,3-di- <i>tert</i> -butyl-2-chloro-1,3,2-diazaphosphorinane $\alpha^{\text{II}}$ a saturated six-membered phosphorus nitrogen heterocycle with a partially flattened chair conformation and a long $\text{P}\cdots\text{Cl}$ bond. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 552-556.	0.2	2
4368	Sonochemical synthesis and crystal structure of dimethylammonium bis[3-carboxy-2-(dimethylamino)propanoato- $\eta^2$ ] $\eta^1$ chloridochromium(II) monohydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 604-606.	0.2	1
4369	Crystal structure and Hirshfeld surface analysis of ( <i>E</i> )-3-[(4-fluorobenzylidene)amino]-5-phenylthiazolidin-2-iminium bromide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 662-666.	0.2	5
4370	The crystal and molecular structures of three copper-containing complexes and their activities in mimicking galactose oxidase. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 538-544.	0.2	1
4371	Crystal structure of <i>N,N</i> -( $\eta^2$ -[(ethane-1,2-diyl)bis(azanediylcarbonothioyl)])bis(benzamide). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 642-645.	0.2	0





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4390	Simulation of diffuse scattering in <sc>DL</sc>-norleucine. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 393-405.	0.5	0
4391	Crystal structure of (<N</i>,<N</i>)-ethylenebis{3-[2-(3-nitrophenyl)hydrazin-1-ylidene]-4-oxopentan-2-iminato}copper(II)-[3-[2-(3-nitrophenyl)hydrazin-1-ylidene]-4-oxopentan-2-iminato]copper(II). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 834-837.		
4392	Crystal structures of the synthetic intermediate 3-[(6-chloro-7H-purin-7-yl)methyl]cyclobutan-1-one, and of two oxetanocin derivatives: 3-[(6-chloro-8,9-dihydro-7H-purin-7-yl)methyl]cyclobutan-1-ol and 3-[(6-chloro-9H-purin-9-yl)methyl]cyclobutan-1-ol. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 732-737.	0.2	1
4393	Crystal structure and Hirshfeld surface analysis of tris(2,2'-bipyridine)nickel(II) bis(1,1,3,3-tetracyano-2-ethoxypropenide) dihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 867-871.	0.2	0
4394	Novel Iron(II) and Copper(II) Polymeric Coordination Compounds with N,N'-bipyridine-type Ligands: Synthesis and Characterization. Chemistry Journal of Moldova, 2019, 14, 120-127.	0.3	1
4395	HBr or not HBr? That is the question: crystal structure of 6-hydroxy-1,4-diazepane-1,4-dium dibromide redetermined. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 678-685.	0.2	0
4396	Potassium chloridotris(hypersiloxy)aluminate dimer. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 714-716.	0.2	1
4397	Bis[<S</i>-benzyl 3-(furan-2-ylmethylidene)dithiocarbazato- <sup>2-</sup> <N</i>]copper(II): crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 794-799.	0.2	2
4398	Synthesis, structure determination and characterization by UV-Vis and IR spectroscopy of bis(diisopropylammonium) <cis</i>-dichloridobis(oxalato- <sup>2-</sup> <O</i>). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 742-745.	0.2	1
4399	Crystal structure, synthesis and thermal properties of tetrakis(4-benzoylpyridine- <sup>1-</sup> <N</i>)bis(isothiocyanato- <sup>1-</sup> <N</i>)iron(II). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 917-920.	0.2	2
4400	Crystal structure of 2<sup>10</sup>-bis(2,6-dichlorophenyl)-4,7,12,15-tetraoxa-2(5,15)-nickel(II)porphyrina-1,3(1,2)-dibenzena-cycloheptadichloromethane monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 925-929.	0.2	0
4401	Crystal structure of a polymorph of <sup>4</sup>-oxido-bis[(5,10,15,20-tetraphenylporphyrinato)iron(III)]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 930-933.	0.2	0
4402	The crystal structures of the ligand <N</i>-(quinolin-8-yl)pyrazine-2-carboxamide and of a tetranuclear copper(II) complex. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 755-761.	0.2	2
4403	Binding of metal ions and water molecules to nucleic acid bases: the influence of water molecule coordination to a metal ion on water-nucleic acid base hydrogen bonds. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 301-309.	0.5	1
4404	Crystal structure of 5-(4-tert-butoxyphenyl)-3-(4-octyloxyphenyl)-4,5-dihydroisoxazole. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 896-899.	0.2	1
4405	Crystal structure of butane-1,4-diyl bis(furan-2-carboxylate). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 872-874.	0.2	0
4406	Crystal structure, DFT and MEP study of (<E</i>)-2-[(2-hydroxy-5-methoxybenzylidene)amino]benzonitrile. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 987-990.	0.2	3
4407	A new tool for finding approximate symmetry. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 835-836.	0.2	3

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4408	(1 <i>R</i> ,2 <i>S</i> ,4 <i>R</i> )-1,2,4-Triphenylcyclopentane-1,2-diol and (1 <i>R</i> ,2 <i>S</i> ,4 <i>R</i> )-4-(2-methoxyphenyl)-1,2-diphenylcyclopentane-1,2-diol: application as initiators for ring-opening polymerization of $\delta$ - $\epsilon$ -caprolactone. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1035-1040.	0.2	0
4409	Synthesis, detailed geometric analysis and bond-valence method evaluation of the strength of $\pi$ -arene bonding of two isotopic cationic prehnitene tin(II) complexes: $[\{1,2,3,4-(\text{CH}_3)_4\text{C}_6\text{H}_2\text{Sn}_2\text{Cl}_2\}][\text{M}]$ ( $\text{M} = \text{Al}$ and $\text{Ga}$ ). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1051-1056.		
4410	Molecular and crystal structure of 5,9-dimethyl-5 <i>H</i> -pyrano[3,2- <i>c</i> :5,6- <i>c'</i> ]-bis[2,1-benzothiazin]-7(9 <i>H</i> )-one 6,6,8,8-tetroxide dimethylformamide monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1076-1078.	0.2	0
4411	Intermolecular hydrogen bonding in isostructural pincer complexes $[\text{OH}(\text{Tj})\text{ETQq1} \cdot 1.0.784314 \text{ rgBT} / \text{Overlock} 10 \text{ Tf} 50 \text{ 627} \text{ Td}]$ . Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1011-1014.	0.2	0
4412	5-Methyl-1,3-phenylene bis[5-(dimethylamino)naphthalene-1-sulfonate]: crystal structure and DFT calculations. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1079-1083.	0.2	0
4413	Structure and Hirshfeld surface analysis of the salt <i>N,N,N</i> -trimethyl-1-(4-vinylphenyl)methanaminium 4-vinylbenzenesulfonate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 946-950.	0.2	1
4414	Synthesis, characterization, and crystal structure of aquabis(4,4'-dimethoxy-2,2'-bipyridine)[ $\frac{1}{4}$ -(2 <i>R</i> ,3 <i>R</i> )-tartrato(4 $\bar{a}$ )]dicopper(II) octahydrate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 972-975.	0.2	1
4415	Crystal structure of ( <i>E</i> )- <i>N</i> -cyclohexyl-2-(2-hydroxy-3-methylbenzylidene)hydrazine-1-carbothioamide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1065-1068.	0.2	0
4416	Crystal structure of <i>N</i> -(diphenylphosphoryl)-2-methoxybenzamide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 939-941.	0.2	0
4417	Crystal structure, spectroscopic characterization and Hirshfeld surface analysis of <i>trans</i> -diaqua[2,5-bis(pyridin-4-yl)-1,3,4-oxadiazole]dithiocyanatonickel(II). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1046-1050.	0.2	1
4418	Crystal structure of 2-(methylamino)tropone. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1128-1132.	0.2	3
4419	A molybdenum tris(dithiolene) complex coordinates to three bound cobalt centers in three different ways. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1261-1264.	0.2	0
4420	7-(Biphenyl-4-yl)-6-hydroxyindan-1-one. IUCrData, 2019, 4, .	0.1	0
4421	Crystal structure of <i>catena</i> -poly[[gold(I)- $\frac{1}{4}$ -cyanido-[diaquabis(2-phenylpyrazine)iron(II)]- $\frac{1}{4}$ -cyanido] dicyanidogold(I)]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1149-1152.	0.2	3
4422	Crystal structure and Hirshfeld surface analysis of ( <i>E</i> )-3-[(4-chlorobenzylidene)amino]-5-phenylthiazolidin-2-iminium bromide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1175-1179.	0.2	1
4423	(3,5-Dimethyladamantan-1-yl)ammonium methanesulfonate (memantinium mesylate): synthesis, structure and solid-state properties. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1274-1279.	0.2	0
4424	Crystal structures of two new isocoumarin derivatives: 8-amino-6-methyl-3,4-diphenyl-1 <i>H</i> -isochromen-1-one and 8-amino-3,4-diethyl-6-methyl-1 <i>H</i> -isochromen-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1117-1122.	0.2	0
4425	Syntheses and structures of piperazin-1-ium $\text{A}(\text{Br})_2$ ( $\text{A} = \text{Cs}$ or $\text{Rb}$ ): hybrid solids containing 'curtain wall' layers of face- and edge-sharing $\text{A}(\text{Br})_6$ trigonal prisms. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1249-1252.	0.2	1

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4426	Di-1/4-acetato-bis{[3-benzyl-1-(2,4,6-trimethylphenyl)imidazol-2-ylidene]silver(I)}. IUCrData, 2019, 4, .	0.1	1
4427	Crystal structures of four dimeric manganese(II) bromide coordination complexes with various derivatives of pyridine <i>N</i> -oxide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1284-1290.	0.2	2
4428	( <i>E</i> )-6,6'-Diazene-1,2-diylbis(1,10-phenanthroline-5-ol) trichloromethane disolvate: a superconjugated ligand. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1224-1227.	0.2	0
4429	Crystal structure of ( <i>E</i> )- <i>N</i> -(3,4-dihydroxybenzylidene)-4-hydroxybenzohydrazide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1280-1283.	0.2	1
4430	Crystal structure and Hirshfeld surface analysis of 2,5-dibromoterephthalic acid ethylene glycol monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1228-1231.	0.2	0
4431	Crystal structure of (15,20-bis(2,3,4,5,6-pentafluorophenyl)-5,10-((pyridine-3,5-diyl)bis((sulfanediy)methylene)[1,1'-biphenyl]-4,4'-diyl))porphyrinato) dichloromethane <i>x</i> -solvate ( <i>x</i> > 1/2) showing a rare CN5 coordination. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1180-1184.	0.2	1
4432	Iodo(triphenyl)silane. IUCrData, 2019, 4, .	0.1	0
4433	Two isomers of [1-benzyl-4-(pyridin-2-yl- <i>N</i> )-1- <i>H</i> -1,2,3-triazole- <i>N</i> ]- <i>Cl</i> <sub>2</sub> ]dichloridobis(dimethyl sulfoxide- <i>S</i> )ruthenium(II). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1108-1111.	0.2	0
4434	Crystal structure, DFT study and Hirshfeld surface analysis of 1-nonyl-2,3-dihydro-1- <i>H</i> -indole-2,3-dione. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1140-1144.	0.2	2
4435	Crystal structure of poly[[ <i>Cl</i> <sub>3</sub> -hydroxido- <i>P</i> ( <i>Cl</i> ) <sub>3</sub> ] [EtQq1 1 0.784314 rgb1 /Overlock 10 11 50 397 1d ( <i>Cl</i> ) <sub>3</sub> ]- <i>N</i> - <i>Cl</i> <sub>2</sub> ]- <i>N</i> - <i>Cl</i> <sub>2</sub> ]- <i>O</i> ]tricopper(II) dihydrate]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1185-1189.	0.2	0
4436	6-Nitro-1,10-phenanthroline-5-amine. IUCrData, 2019, 4, .	0.1	0
4437	Crystal structure of a low-spin poly[di-1/4-cyanido-di-1/4-cyanido-bis(1/4-2-ethylpyrazine)dicopper(I)iron(II)]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1205-1208.		0
4438	Bis(mefloquinium) butanedioate ethanol monosolvate: crystal structure and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1162-1168.	0.2	0
4439	Steric and electronic evaluations of P( <i>o</i> - <i>R</i> ) <sub>2</sub> , where <i>R</i> is phenyl or cyclohexyl: crystal structures of SeP( <i>o</i> - <i>R</i> ) <sub>2</sub> . Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 1310-1318.	0.2	0
4440	Deciphering the hydrogen-bonding scheme in the crystal structure of triphenylmethanol: a tribute to George Ferguson and co-workers. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 1266-1273.	0.2	2
4441	Synthesis and structure of push-pull merocyanines based on barbituric and thiobarbituric acid. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1306-1310.	0.2	1
4442	Crystal structure of tetramethylammonium 1,1,7,7-tetracyanohepta-2,4,6-trienide. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1344-1347.	0.2	0
4443	Synthesis, characterization, crystal structure and supramolecularity of ethyl ( <i>E</i> )-2-cyano-3-(3-methylthiophen-2-yl)acrylate and a new polymorph of ethyl ( <i>E</i> )-2-cyano-3-(thiophen-2-yl)acrylate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1357-1361.	0.2	4

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4444	Crystal structure and magnetic properties of bis[butyltris(1 <i>H</i> -pyrazol-1-yl)borato]iron(II). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1327-1330.	0.2	0
4446	Crystal structure and Hirshfeld surface analysis of lapachol acetate 80 years after its first synthesis. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1362-1366.	0.2	0
4447	Crystal structure of a binuclear mixed-valence ytterbium complex containing a 2-anthracene-substituted phenoxide ligand. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1367-1371.	0.2	0
4448	The first crystal structure of the pyrrolo[1,2- <i>c</i> ]oxazole ring system. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1336-1338.	0.2	1
4449	<i>N</i> -Tosyl-L-proline benzene hemisolvate: a rare example of a hydrogen-bonded carboxylic acid dimer with symmetrically disordered H atoms. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 1228-1233.	0.2	2
4450	Crystal structure and Hirshfeld surface analysis of 4-(4-methylbenzyl)-6-phenylpyridazin-3(2 <i>H</i> )-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1352-1356.	0.2	6
4451	Synthesis and crystal structure of <i>tert</i> -butyl 1-(2-iodobenzoyl)cyclopent-3-ene-1-carboxylate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1383-1385.	0.2	0
4452	Crystal structure of (E)-3-(2-hydroxy-4-methylphenyl)-1-(2,4,6-trimethoxyphenyl)prop-2-en-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1379-1382.	0.2	1
4453	Absolute structure of (3 <i>S</i> ,5 <i>S</i> ,7 <i>aS</i> ,7 <i>bS</i> ,9 <i>aR</i> ,10 <i>R</i> ,12 <i>aR</i> ,12 <i>bS</i> )-7 <i>b</i> -hydroxy-4,4,7 <i>a</i> ,9 <i>a</i> ,12 <i>a</i> -pentamethyl-10-oxo-1,2,3,4,5,6,7,8,9,10,11,12-dodecahydro-1 <i>H</i> -indole-1,2-dione. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1348-1351.	0.2	0
4454	Syntheses and crystal structures of 2-methyl-1,1,2,3,3-pentaphenyl-2-silapropane and 2-methyl-1,1,3,3-tetraphenyl-2-silapropan-2-ol. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1339-1343.	0.2	0
4455	Synthesis, structure and hydrogen sorption properties of a pyrazine-bridged copper(I) nitrate metal-organic framework. European Journal of Chemistry, 2019, 10, 195-200.	0.3	2
4456	Crystal structures of 3-chloro-2-nitrobenzoic acid with quinoline derivatives: 3-chloro-2-nitrobenzoic acid $\pi$ -5-nitroquinoline (1/1), 3-chloro-2-nitrobenzoic acid $\pi$ -6-nitroquinoline (1/1) and 8-hydroxyquinolinium 3-chloro-2-nitrobenzoate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1552-1557.	0.2	4
4457	The crystal structure of ((cyclohexylamino){(E)-2-[(E)-5-methoxy-3-nitro-2-oxidobenzylidene- $\eta^5$ -O]hydrazin-1-ylidene- $\eta^5$ -N} Tj ETQq0 0 O two-dimensional network. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1486-1489.	0.2	2
4458	The crystal structures and Hirshfeld surface analyses of four 3,5-diacetyl-2-methyl-2,3-dihydro-1,3,4-thiadiazol-2-yl derivatives. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1436-1444.	0.2	0
4459	The crystal structure of the zwitterionic co-crystal of 2,4-dichloro-6-[(3-hydroxypropyl)azaniumyl]methyl}phenolate and 2,4-dichlorophenol. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1452-1455.	0.2	0
4460	Crystal structure of 4-bromo-N-[(3,6-di- <i>tert</i> -butyl-9 <i>H</i> -carbazol-1-yl)methylidene]aniline. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1429-1431.	0.2	0
4461	Crystal structure of <i>catena</i> -poly[[[bis(3-oxo-1,3-diphenylprop-1-enolato- $\eta^2$ ) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 1 <i>N,N'</i> -tetrahydrofuran monosolvate]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1432-1435.	0.2	0
4463	Crystal structure of poly[[diaquatetra- $\eta^4$ -cyanido-iron(II)platinum(II)] acetone disolvate]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1536-1539.	0.2	1







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4482	Synthesis and crystal structure of (<i>E</i>)-2-({2-[azaniumylidene(methylsulfanyl)methyl]hydrazinylidene}methyl)benzene-1,4-diol hydrogen sulfate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1738-1740.	0.2	0
4483	Crystal structures of 2-(2-bromo-5-fluorophenyl)-8-ethoxy-3-nitro-2<i>H</i>-thiochromene and 2-(2-bromo-5-fluorophenyl)-7-methoxy-3-nitro-2<i>H</i>-thiochromene. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1783-1786.	0.2	2
4484	Synthesis and crystal structure of (<i>E</i>)-1,2-bis[2-(methylsulfanyl)phenyl]diazene. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1808-1811.	0.2	0
4485	Crystal structure and Hirshfeld surface analysis of 2,2â€²-[(1<i>E</i>),1â€²<i>E</i>]-[ethane-1,2-diylbis(azanylylidene)]bis(methanylylidene)bis[4-(trifluoromethoxy)phenol]copper(II) hydroquinone hemisolvate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1729-1733.	0.2	0
4486	Crystal structures of the two isomeric hydrogen-bonded cocrystals 2-chloro-4-nitrobenzoic acidâ€²5-nitroquinoline (1/1) and 5-chloro-2-nitrobenzoic acidâ€²5-nitroquinoline (1/1). Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1694-1699.	0.2	4
4487	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of (2<i>Z</i>)-4-benzyl-2-(2,4-dichlorobenzylidene)-2<i>H</i>-1,4-benzothiazin-3(4<i>H</i>)-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1650-1656.	0.2	3
4488	Crystal structure and Hirshfeld surface analysis of (<i>E</i>)-6-(4-hydroxy-3-methoxystyryl)-4,5-dihydropyridazin-3(2<i>H</i>)-one. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1734-1737.	0.2	5
4489	Crystal structures, syntheses, and spectroscopic and electrochemical measurements of two pushâ€²pull chromophores: 2-[4-(dimethylamino)benzylidene]-1<i>H</i>-indene-1,3(2<i>H</i>)-dione and (<i>E</i>)-2-[3-[4-(dimethylamino)phenyl]allylidene]-1<i>H</i>-indene-1,3(2<i>H</i>)-dione. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1595-1599.	0.2	3
4490	Crystal structure and mesogenic behaviour of a new fluorene derivative: 9,9-dimethyl-2,7-bis(4-pentylphenyl)-9<i>H</i>-fluorene. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 1459-1464.	0.2	1
4491	The crystal structures of two novel polymorphs of bis(oxonium) ethane-1,2-disulfonate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1586-1589.	0.2	1
4492	Tetra<i>n</i>-butylammonium orotate monohydrate: knowledge-based comparison of the results of accurate and lower-resolution analyses and a non-routine disorder refinement. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1632-1637.	0.2	1
4493	Different packing motifs mediated by weak interactions and polymorphism in the crystal structures of five 2-(benzylidene)benzosuberone derivatives. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1741-1747.	0.2	0
4494	Crystal structure and Hirshfeld surface analysis of (2<i>E</i>)-2â€²<i>E</i>-1,1â€²-[selenobis(4,1-phenylene)]bis[3-(4-chlorophenyl)prop-2-en-1-one]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1724-1728.	0.2	1
4495	Crystal structure of benzyl <i>N</i>-â€²-[(1<i>E</i>),4<i>E</i>]-1,5-bis(4-methoxyphenyl)penta-1,4-dien-3-ylidene]hydrazine-1-carbodithioate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1613-1619.	0.2	1
4496	Synthesis and structure of 2,4,6-tricyclobutyl-1,3,5-trioxane. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1578-1581.	0.2	0
4497	The 'super acid' BF<sub>3</sub>H<sub>2</sub>O stabilized by 1,4-dioxane: new preparative aspects and the crystal structure of BF<sub>3</sub>H<sub>2</sub>Oâ€²C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1787-1791.	0.2	5
4498	Crystal structure of <i>catena</i>-poly[[[(2-ethoxypyrazine-â€²<i>N</i>)copper(I)]-di-â€²<sub>2</sub>-cyanido][copper(I)-â€²<sub>2</sub>-cyanido]]. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1797-1800.	0.2	0
4499	Crystal structure, computational study and Hirshfeld surface analysis of ethyl (2<i>S</i>)-3<i>R</i>-3-(3-amino-1<i>H</i>-1,2,4-triazol-1-yl)-2-hydroxy-3-phenylpropanoate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1919-1924.	0.2	1



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4518	The first coordination compound of deprotonated 2-bromonicotinic acid: crystal structure of a dinuclear paddle-wheel copper(II) complex. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 225-230.	0.2	1
4519	Crystal structure, synthesis and thermal properties of bis(4-benzoylpyridine- $\hat{p}$ -N</i>)bis(isothiocyanato- $\hat{p}$ -N</i>)bis(methanol- $\hat{p}$ -N</i>)iron(II). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 276-280.	0.2	0
4520	Chromium complexes bearing disubstituted organophosphate ligands and their use in ethylene polymerization. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 93-103.	0.2	1
4521	Powder X-ray diffraction of flucytosine, C <sub>4</sub> H <sub>4</sub> FN <sub>3</sub> O. <i>Powder Diffraction</i> , 2020, 35, 67-68.	0.4	0
4522	Crystal structure and Hirshfeld surface analysis of 1,2,4-triazolium hydrogen oxalate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 137-140.	0.2	1
4523	Synthesis and crystal structures of a bis(3-hydroxy-cyclohex-2-en-1-one) and two hexahydroquinoline derivatives. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 125-131.	0.2	3
4524	Twist-chair conformation of the tetraoxepane ring remains unchanged in tetraoxaspirododecane diamines. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 276-286.	0.2	4
4525	Crystal structure of a nickel compound comprising two nickel(II) complexes with different ligand environments: [Ni(tren)(H<sub>2</sub>O)<sub>2</sub>][Ni(H<sub>2</sub>O)<sub>6</sub>](SO<sub>4</sub>)<sub>2</sub>. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 314-317.	0.2	1
4526	Synthesis and Structure of [Fe <sub>3</sub> ( $\hat{p}$ -Q)( $\hat{p}$ -3-AsN(i-Bu) <sub>2</sub> )(CO) <sub>9</sub> ] (Q = Se, Te) Clusters and Products of Their Hydrolysis. <i>Journal of Structural Chemistry</i> , 2020, 61, 283-292.	0.3	0
4527	Bulky 2,6-disubstituted aryl siloxanes and a disilanamine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 318-323.	0.2	1
4528	The crystal structures and Hirshfeld surface analyses of a cadmium(II) and a zinc(II) mononuclear complex of the new tetrakis-substituted pyrazine ligand <i>N</i>,<i>N</i>â€²,<i>N</i>â€²â€²,<i>N</i>â€²â€²â€²-[pyrazine-2,3,5,6-tetrayltetrakis(methylene)]tetrakis(<i>N</i>-methyl)aniline). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 410-416.	0.2	0
4529	Crystal structure and Hirshfeld surface analysis of 3,6-bis(pyrimidin-2-yl)-1,4-dihydro-1,2,4,5-tetrazine dihydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 473-476.	0.2	0
4530	Crystal structure and Hirshfeld surface analysis of 3,4-dihydro-2<i>H</i>-anthra[1,2-<i>b</i>][1,4]dioxepine-8,13-dione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 576-580.	0.2	0
4531	Crystal structure and Hirshfeld surface analysis of hexyl 1-hexyl-2-oxo-1,2-dihydroquinoline-4-carboxylate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 642-645.	0.2	0
4532	Synthesis and crystal structures of tetrameric [2-(4,4-dimethyl-2-oxazolin-2-yl)anilido]sodium and tris[2-(4,4-dimethyl-2-oxazolin-2-yl)anilido]ytterbium(III). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 703-709.	0.2	0
4533	Sodium sulfite heptahydrate and its relation to sodium carbonate heptahydrate. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 427-432.	0.2	1
4534	Polymorphism and phase transformation in the dimethyl sulfoxide solvate of 2,3,5,6-tetrafluoro-1,4-diiodobenzene. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 524-529.	0.2	0
4535	Crystal structure of bis(1-mesityl-1<i>H</i>-imidazole- $\hat{p}$ -N</i> <sup>3</sup>)diphenylboron trifluoromethanesulfonate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 673-676.	0.2	2

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4536	Crystal structures of {1,1,1-tris[(salicylaldimino)methyl]ethane}gallium as both a pyridine solvate and an acetonitrile 0.75-solvate and {1,1,1-tris[(salicylaldimino)methyl]ethane}indium dichloromethane solvate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 615-620.	0.2	0
4537	Crystal structure of <i>trans</i> -dichlorido(1,4,8,11-tetraazacyclotetradecane- $\eta^4$ ) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Crystallographic Communications, 2020, 76, 656-659.	0.2	0
4538	The missing crystal structure in the series of $\epsilon$ , $\epsilon$ -tris(pyridinyl)benzene-1,3,5-tricarboxamides: the 2-pyridinyl derivative. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 776-779.	0.2	0
4539	Crystal structure, Hirshfeld surface analysis and computational study of the 1:2 co-crystal formed between $\epsilon$ -bis[(pyridin-4-yl)methyl]ethanediamide and 3-chlorobenzoic acid. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 870-876.	0.2	0
4540	The crystal structure and Hirshfeld surface analysis of 1-(2,5-dimethoxyphenyl)-2,2,6,6-tetramethylpiperidine. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 794-797.	0.2	0
4541	The Zn( <i>S</i> -pr-thiosal) <sub>2</sub> complex attenuates murine breast cancer growth by inducing apoptosis and G1/S cell cycle arrest. Future Medicinal Chemistry, 2020, 12, 897-914.	1.1	7
4542	Crystal structure, Hirshfeld surface analysis and interaction energy, DFT and antibacterial activity studies of ( <i>Z</i> )-4-hexyl-2-(4-methylbenzylidene)-2 <i>H</i> -benzo[1,4]thiazin-3(4 <i>H</i> )-one. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 889-895.	0.2	0
4543	Crystal structure of a 1:1 co-crystal of the anticancer drug gefitinib with azelaic acid. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 884-888.	0.2	1
4545	Febuxostat ethanol monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 816-819.	0.2	0
4546	Molecular and crystal structure, optical properties and DFT studies of 1,4-dimethoxy-2,5-bis[2-(4-nitrophenyl)ethenyl]benzene. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 940-943.	0.2	0
4547	Hydrothermal synthesis and crystal structure of poly[bis( $\eta^3$ -3,4-diaminobenzoato)manganese], a layered coordination polymer. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 909-913.	0.2	0
4548	Synthesis and crystal structure of (1,10-phenanthroline) $\eta^2$ Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 312 Td ( <i>N</i> ) <sub>2</sub> <sup>+</sup> iridium(III) hexafluoridophosphate with an unknown number of solvent molecules. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 803-806.	0.2	1
4549	Crystal structure of <i>catena</i> -poly[[[diaqua[1,2-bis(pyridin-4-yl)ethene]{4-[2-(pyridin-4-yl)ethenyl]pyridinium}gold(I)iron(II)]-di( $\eta^4$ -cyanido)bis[dicyanidogold(I)] 1,2-bis(pyridin-4-yl)ethene dihydrate]. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 944-947.	0.2	0
4550	Crystal structure of a cadmium sulfate coordination polymer based on the 3,6-bis(pyrimidin-2-yl)-1,4-dihydro-1,2,4,5-tetrazine ligand. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 958-961.	0.2	0
4551	Crystal structure of dimethyl 5-(4-ethylphenyl)-4-[(4-ethylphenyl)ethynyl]-6,11-diphenyl-1,3,6,11-tetrahydro-2 <i>H</i> -6,11-epoxycyclopenta[ <i>a</i> ]anthracene-2,2-dione. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 954-957.	0.2	0
4552	Crystal structure and characterization of a new copper(II) chloride dimer with methyl(pyridin-2-ylmethylidene)amine. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 790-793.	0.2	0
4553	Synthesis and crystal structure of two manganese-based 12-metallacrown-4 complexes: Na <sub>2</sub> (3-chlorobenzoate) <sub>2</sub> [12-MC <sub>2</sub> Mn(III)N(shi) <sub>4</sub> ](DMF) <sub>6</sub> and MnNa(3-chlorobenzoate) <sub>3</sub> [12-MC <sub>2</sub> Mn(III)N(shi) <sub>4</sub> ](DMF)(H <sub>2</sub> O) <sub>4</sub> ·4DMF·0.72H <sub>2</sub> O. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 848-856.	0.2	0
4554	Diammonium potassium citrate, (NH <sub>4</sub> ) <sub>2</sub> K <sub>6</sub> H <sub>5</sub> O <sub>7</sub> . IUCrData, 2020, 5, .	0.1	2



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4555	2- <i>O</i> -Monoalkyl isosorbide ethers with C8, C10, C12 and C14 chain lengths. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 924-928.	0.2	0
4556	Crystal structures of 6-cyclopropyl-1,3-diphenylfulvene and 6-(2,3-dimethoxynaphthyl)-1,3-diphenylfulvene. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 896-899.	0.2	0
4557	Stereochemistry of the methylidene-bridged quinazoline-isoquinoline alkaloid 3-[[6,7-dimethoxy-1-(4-nitrophenyl)-1,2,3,4-tetrahydroisoquinolin-2-yl]methylidene]-1,2,3,9-tetrahydropyrrolo[2,1- <i>b</i> ]quinazolin-9-methanol monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 914-919. <i>Synthesis, crystal structures, topology and photoluminescent properties of</i>	0.2	1
4558	<i>poly</i> [di- $\frac{1}{4}$ -aqua-diaqua[ $\frac{1}{4}$ - $\text{H}$ -tetrazol-1-id-5-yl]benzoato- $\text{P}^{\text{O}}$ ] <sup>4-</sup> and <i>poly</i> [ $\frac{1}{4}$ -aqua-diaqua[ $\frac{1}{4}$ - $\text{H}$ -tetrazol-1-id-5-yl]benzoato- $\text{P}^{\text{O}}$ ] <sup>4-</sup> <i>strontium(II)</i> . Acta Crystallographica Section E: Crystallographic	0.2	0
4559	Crystal structures of two isostructural compounds: a second polymorph of dipotassium hydrogen citrate, $\text{K}_2\text{HC}_6\text{H}_5\text{O}_7$ , and potassium rubidium hydrogen citrate, $\text{KRbHC}_6\text{H}_5\text{O}_7$ . Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 706-715.	0.2	1
4560	Hydrogen atom disorder in the crystal structure of <i>o</i> -phenylenediacetic acid. Nova Biotechnologica Et Chimica, 2020, 19, 109-115.	0.1	0
4561	Crystal structure and Hirshfeld surface analysis of 4-[2,2-dichloro-1-[( <i>E</i> )-(4-chlorophenyl)diazanyl]ethenyl]- <i>N,N</i> -dimethylaniline. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1033-1037.	0.2	2
4562	Polymorphism of bis(1,3-benzothiazol-2-yl) trithiocarbonate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1126-1130.	0.2	0
4563	Reactivity trends of cobalt(III) complexes towards various amino acids based on the properties of the amino acid alkyl chains. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 663-672.	0.2	2
4564	Crystal structure of <i>N,N</i> -diisopropyl-4-methylbenzenesulfonamide. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1018-1021.	0.2	0
4565	Reductive cleavage of <i>N,N</i> -di- <i>tert</i> -butylcarbodiimide generates <i>tert</i> -butylcyanamide ligands, $(\text{Me}_3\text{CNCN})^{\text{O}}$ , that bind potassium both end-on and side-on in the same single crystal. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1047-1050.	0.2	0
4566	Crystal structure and Hirshfeld surface analysis of one-dimensional copper(II) coordination polymer incorporating succinate and tetramethylethylenediamine ligands. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1038-1041.	0.2	1
4567	Synthesis, structure and biological activity of four new picolinohydrazoneamide derivatives. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 673-680.	0.2	2
4568	Crystal structures and Hirshfeld surface analyses of 6,8-dimethoxy-3-methyl-1- <i>H</i> -isochromen-1-one and 5-bromo-6,8-dimethoxy-3-methyl-1- <i>H</i> -isochromen-1-one chloroform monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1107-1112.	0.2	0
4569	Crystal structure and Hirshfeld surface analysis of 1-methyl-4-(2-methyl-10- <i>H</i> -benzo[ <i>b</i> ]thieno[2,3- <i>e</i> ][1,4]diazepin-4-yl)piperazin-1-ium 2,5-dihydroxybenzoate propan-2-ol monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1168-1172.	0.2	0
4570	The crystal structures, Hirshfeld surface analyses and energy frameworks of two hexathiapyrazinophane regioisomers; 2,5,8,11,14,17-hexathia-[9.9](2,6,3,5)-pyrazinophane and 2,5,8,11,14,17-hexathia-[9.9](2,5,3,6)-pyrazinophane. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 977-983.	0.2	1
4571	Crystal structure and Hirshfeld surface analysis of 2-[[4-iodophenyl]imino]methyl]-4-nitrophenol. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1146-1149.	0.2	3
4572	Crystallographic and spectroscopic characterization of racemic Mosher's Acid. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1143-1145.	0.2	0

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4573	Crystal structure of the [(THF)Cs( $\frac{1}{4}$ - $\lambda$ <sup>5</sup> : $\lambda$ <sup>5</sup> -Cp $\epsilon^2$ ) <sub>3</sub> Yb] <sub>n</sub> oligomer. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1131-1135.	0.2	1
4574	Synthesis and crystal structures of 3-hydroxy-2,4-dimethyl-2H-thiophen-5-one and 3-hydroxy-4-methyl-2H-thiophen-5-one. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1158-1162.	0.2	0
4575	Crystal structure and Hirshfeld surface analysis of the orthorhombic polymorph of a Zn <sup>II</sup> complex with 3,5-dinitrobenzoic acid and ethylenediamine. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1113-1116.	0.2	1
4576	The conformational analyses of 2-amino-N-[2-(dimethylphenoxy)ethyl]propan-1-ol derivatives in different environments. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 681-689.	0.2	1
4577	Crystal structure and Hirshfeld surface analysis of 1-(2-fluorophenyl)-1H-tetrazole-5(4H)-thione. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1007-1011.	0.2	6
4578	Di( $\frac{1}{4}$ -aqua-bis[aqua(2,2 $\epsilon^2$ -bipyridine)(4-nitrobenzoato)cobalt(II)] bis(4-nitrobenzoate). IUCrData, 2020, 5, .	0.1	2
4579	Crystal structure, Hirshfeld surface analysis and DFT studies of ( <i>E</i> )-4-methyl-2-[(4-methylphenyl)imino]methylphenol. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1075-1079.	0.2	0
4580	Crystal structure and Hirshfeld surface analysis of 4-[[( <i>E</i> )-4-(heptyloxy)benzylidene]amino]-N-(naphthalen-2-yl)-1,3-thiazol-2-amine. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1092-1095.	0.2	0
4581	Crystal structures of [( $\frac{1}{4}$ -L1) <sub>2</sub> dibromidodicopper(II)] dibromide and poly[[( $\frac{1}{4}$ -L1) <sub>2</sub> diiodidodicopper(I)]-di( $\frac{1}{4}$ -iodido-dicopper(I)), where L1 is 2,5,8,11,14,17-hexathia-[9.9](2,6,3,5)-pyrazinophane. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 984-989.	0.2	1
4582	( <i>E</i> )-2-(3,5-Dimethoxybenzylidene)indan-1-one. IUCrData, 2020, 5, .	0.1	1
4583	The crystal structure, Hirshfeld surface analysis and energy frameworks of 2-[2-(methoxycarbonyl)-3,6-bis(methoxymethoxy)phenyl]acetic acid. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1101-1106.	0.2	0
4584	The low-temperature triclinic crystal structure of silver 3-sulfobenzoic acid. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1275-1278.	0.2	1
4585	Bis(3,5-dinitrobenzoato- $\eta^{\circ}$ O) <sub>2</sub> bis(ethane-1,2-diamine- $\lambda^2$ : $\lambda^2$ -N,N $\epsilon^2$ )cadmium(II). IUCrData, 2020, 5, .	0.1	0
4586	Synthesis, crystal structures and Hirshfeld surface analysis of 1,4-dibenzyl-6-methyl-1,4-dihydroquinoxaline-2,3-dione. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1361-1364.	0.2	1
4587	Diaquabis( $\frac{1}{4}$ -1,5-bis[(pyridin-2-yl)methylidene]carbonohydrazide(1 $\epsilon^+$ ))di( $\frac{1}{4}$ -chlorido-tetrachloridotetrazinc(II)). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1349-1352.	0.2	0
4588	Crystal structures of two isostructural bivalent metal N-benzoylglycinates. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1260-1265.	0.2	0
4589	Crystal structure, Hirshfeld surface analysis and DFT studies of 4-methyl-2-([4-(trifluoromethyl)phenyl]imino)methylphenol. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1325-1330.	0.2	2
4590	Syntheses and crystal structures of solvate complexes of alkaline earth and lanthanoid metal iodides with N,N-dimethylformamide. Zeitschrift Fur Kristallographie - Crystalline Materials, 2020, 235, 401-411.	0.4	4



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4591	Synthesis by deamination reaction and crystal structure at 120 K of (1 <i>Z</i> ,19 <i>E</i> )-18-oxo-1 <i>N</i> -(pyridin-2-yl)-6,7,9,10-tetrahydro-18 <i>H</i> -dibenzo[ <i>h</i> , <i>o</i> ][1,4,7]trioxacyclohexane. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1454-1457.	0.2	1
4592	High-pressure preference for reduced water content in porous zinc aspartate hydrates. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 795-801.	0.5	0
4593	(1 <i>R</i> ,3 <i>S</i> )-3-(1 <i>H</i> -Benzo[ <i>d</i> ]imidazol-2-yl)-1,2,2-trimethylcyclopentane-1-carboxylic acid as a new anti-diabetic active pharmaceutical ingredient. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1407-1411.	0.2	1
4594	4-Styrylquinolines from cyclocondensation reactions between (2-aminophenyl)chalcones and 1,3-diketones: crystal structures and regiochemistry. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 883-890.	0.2	4
4595	A rare octacoordinated mononuclear iron(III) spin-crossover compound: synthesis, crystal structure and magnetic properties. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 856-862.	0.2	0
4596	Crystal structures of [( <i>N,N</i> -dimethylamino)methyl]ferrocene and ( <i>R</i> ) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1437-1441.	0.2	1
4597	Combining valproate and bipyridyl ligands to construct a 0D core-shell Zn <sub>5</sub> (1/4 <sub>3</sub> -OH) <sub>2</sub> cluster and a 2D layered coordination network with a [Zn <sub>3</sub> (1/4 <sub>3</sub> -OH)] <sub>2</sub> SBU. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 897-906.	0.2	0
4598	Influence of meso-linker attachment on the formation of core- $\pi$ interactions in urea-functionalized porphyrins. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2020, 75, 755-764.	0.3	0
4599	Crystal structure and Hirshfeld surface analysis of 4-aminopyridinium thiocyanate $\cdot$ 4-aminopyridine (1/1). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1535-1538.	0.2	5
4600	Crystal structure and Hirshfeld analysis of 3-bromo-4-methylchalcone and 3-cyano-4-methylchalcone. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1496-1502.	0.2	1
4601	Crystal structure of bis[( <i>R,R</i> )-1,2-(binaphthylphosphonito)ethane]dichloridoiron(II) dichloromethane disolvate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1525-1527.	0.2	1
4602	Structural (at 100 K) and DFT studies of 2-nitroflavone. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1417-1420.	0.2	0
4603	Synthesis, crystal structure and Hirshfeld surface analysis of 1,7-dimethyl-5 <i>a</i> ,6,11 <i>a</i> ,12-tetrahydrobenzo[ <i>b</i> ]benzo[5,6][1,4]oxazino[2,3- <i>e</i> ][1,4]oxazine. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1472-1475.	0.2	2
4604	Layered alkali propanoates $\text{M}^+(\text{C}_2\text{H}_5\text{COO})_2$ ; $\text{M}^+ = \text{Na}^+, \text{K}^+, \text{Rb}^+, \text{Cs}^+$ . Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1508-1513.	0.2	1
4605	Synthesis and structures of three isoxazole-containing Schiff bases. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 927-931.	0.2	0
4606	Revisiting the absolute chirality and polymorphism of ( $\alpha$ )-Istanbulin A. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 914-920.	0.2	1
4607	Crystal structure of bis( <i>N,N</i> - $\beta$ -dimethylthiourea- $\beta$ - <i>S</i> )bis(thiocyanato- $\beta$ - <i>N</i> )cobalt(II). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1476-1481.	0.2	1
4608	4,15-Dimethyl-7,12-diazoniatricyclo[10.4.0.0 <sup>2,7</sup> ]hexadeca-1(12),2,4,6,13,15-hexaene dibromide monohydrate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1467-1471.	0.2	0



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4627	Homo- and heterometallic oxalate-based complexes obtained using $[\text{Cr}(\text{C}_2\text{O}_4)_3]^{3-}$ building block – two polymorphs of a solvate. <i>Polyhedron</i> , 2021, 211, 115556.	1.0	1
4628	Crystal structure, Hirshfeld surface and frontier molecular orbital analysis of 9-(3-bromo-4-hydroxy-5-methoxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1 <i>H</i> -xanthene-1,8(2 <i>H</i> )-dione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 1170-1174.		
4629	Crystal structures of $\text{Zn}(\text{cyclam})\text{I}^{2+}$ (second monoclinic polymorph) and $\text{Zn}(\text{cyclam})\text{I}^{3+}$ . <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 1185-1189.	0.2	3
4630	Manganese(I) tricarbonyl complexes as potential anticancer agents. <i>Journal of Biological Inorganic Chemistry</i> , 2022, 27, 49-64.	1.1	4
4631	Unraveling the Origins of Strong and Reversible Chemisorption of Carbon Dioxide in a Green Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2021, 125, 24719-24727.	1.5	9
4632	Synthesis and crystal structure of (1,8-naphthyridine) <sup>2+</sup> Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 552 Td (<i>N</i>)<sup>1</sup>iridium(III) hexafluoridophosphate dichloromethane monosolvate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 82-85.	0.2	0
4633	An indenide-tethered N-heterocyclic stannylene. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 254-256.	0.2	2
4634	Crystal and Molecular Structure Analysis in Knoevenagel Condensation Product of Substituted Naphthofuran-2-Carbaldehydes. <i>Crystal Structure Theory and Applications</i> , 2020, 09, 49-62.	0.3	0
4635	Sparfloxacin Multicomponent Crystals: Targeting the Solubility of Problematic Antibiotics. <i>Crystal Growth and Design</i> , 2021, 21, 995-1005.	1.4	9
4636	Chemo- and Stereospecific Solid-State Thermal Dimerization of Sodium trans-2-Butenoate and $\beta$ -Ray-Induced Single-Crystal-to-Single-Crystal Dimerization of Hexaaquamagnesium trans-2-Butenoate Dihydrate: Both Give rel-(3 <i>S</i> ,4 <i>R</i> )-1-Hexene-3,4-dicarboxylate but by Different Mechanisms. Stereospecific $\beta$ -Ray-Induced Trimerization of Sodium trans-2-Butenoate. <i>Crystal Growth and Design</i> , 2021, 21, 663-682.	1.4	2
4637	New Polymorph of Tetrakis(pentafluorophenyl)diboroxane (C <sub>6</sub> F <sub>5</sub> ) <sub>2</sub> BOB(C <sub>6</sub> F <sub>5</sub> ) <sub>2</sub> . <i>Russian Journal of General Chemistry</i> , 2020, 90, 2528-2530.	0.3	0
4638	Reversible Phase Transition in the MoO <sub>2</sub> Cl <sub>2</sub> (DME) Structure with the Retention of the Crystal System and Space Group. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2020, 46, 812-816.	0.3	1
4639	Single-crystal X-ray structure determinations of vardenafil, vardenafil dihydrate, vardenafil monohydrochloride trihydrate and vardenafil dihydrochloride hexahydrate. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2021, 76, 45-53.	0.3	0
4640	Crystal Structure Prediction; From the Present to the Future. <i>Nihon Kessho Gakkaishi</i> , 2020, 62, 260-268.	0.0	1
4641	The interaction between $[\text{Pt}(\text{Safrole-1H})_2]$ and 1,3-diisopropylbenzimidazolium bromide in the presence of Ag <sub>2</sub> O. <i>Science and Technology</i> , 2020, 58, 728-735.	0.1	1
4642	The incidence of kryptoracemic crystallization in $[\text{CoIII}(\text{tren})\text{XY}]^+$ compounds: The case of cis- $[\text{CoIII}(\text{tren})\text{Cl}_2]\text{Cl}\cdot\text{H}_2\text{O}$ . <i>European Journal of Chemistry</i> , 2020, 11, 314-318.	0.3	0
4643	Building Up Co-Crystals: Structural Motif Consistencies Across Families of Co-Crystals. <i>Proceedings (mdpi)</i> , 2021, 78, 45.	0.2	0
4644	1,7,7-Trimethyl-3-(naphthalen-2-ylcarbonyl)bicyclo[2.2.1]heptan-2-one. <i>IUCrData</i> , 2020, 5, .	0.1	0

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4645	Comparative Study of Chalcones and Their Potential as Additives for Biofuels. <i>Energy &amp; Fuels</i> , 2021, 35, 552-560.	2.5	6
4646	Amino acid hydrogen oxalate quasiracemates with sulfur containing side chains. <i>CrystEngComm</i> , 2021, 23, 8061-8070.	1.3	1
4647	Ionic liquids for renewable thermal energy storage – a perspective. <i>Green Chemistry</i> , 2022, 24, 102-117.	4.6	34
4648	Near-infrared absorbing hydrogen-bonded dithioketopyrrolopyrrole (DTPP) n-type semiconductors. <i>Dyes and Pigments</i> , 2022, 197, 109884.	2.0	7
4649	Homobinuclear compounds based on a chiral oxazolidine ligand: From solid state study to aqueous solution dynamics. <i>Inorganica Chimica Acta</i> , 2022, 529, 120664.	1.2	1
4650	Cyclopentadienyl lanthanide borohydrides derived from the unsubstituted cyclopentadienyl ligand. Unprecedented structural diversity and $\mu$ -caprolactone polymerization. <i>Inorganica Chimica Acta</i> , 2022, 529, 120638.	1.2	2
4651	From $\eta^3$ - to $\eta^4$ - agostic methyl coordination: NMR and solid state study of donor ligands uptake by the triangular cluster anion $[\text{Re}_3(\eta^4\text{-H})_3(\eta^3\text{-CH}_3)(\text{CO})_9]^-$ . <i>Inorganica Chimica Acta</i> , 2022, 529, 120641.	1.2	0
4652	A cross-phase reaction coordinate in the formation of a simple copper (II) orotate complex: Lability of crystals of a Jahn-Teller active intermediate. <i>Journal of Molecular Structure</i> , 2022, 1249, 131640.	1.8	0
4653	Iodonium Polyiodide Crystals in the Framework of Periodic Calculations with Localized Atomic Basis Sets. <i>Bulletin of the South Ural State University Series Chemistry</i> , 2020, 12, 101-109.	0.3	0
4654	A new heteroleptic phosphorescent cuprous complex supported by a BINAP ligand: synthesis, structure, luminescence properties and theoretical analyses. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 177-185.	0.2	4
4655	Crystal and molecular structures of a binuclear mixed ligand complex of silver(I) with thiocyanate and 1 <i>H</i> -1,2,4-triazole-5(4 <i>H</i> )-thione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 42-47.	0.2	0
4656	A simple and high-yield route to iridium, rhodium, osmium and ruthenium <i>nido</i> -6-metalladecaborane compounds. <i>Dalton Transactions</i> , 2021, 50, 16751-16764.	1.6	3
4657	Triel bonds within anion $\text{B}^-\text{B}^-\text{B}^-$ anion complexes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25097-25106.	1.3	6
4658	Dinitrogen Binding and Functionalization. , 2022, , 521-554.		5
4659	Crystal structure, Hirshfeld surface analysis and PIXEL calculations of a 1:1 epimeric mixture of 3-[(4-nitrobenzylidene)amino]-2( <i>R,S</i> )-(4-nitrophenyl)-5( <i>S</i> )-(propan-2-yl)imidazolidin-4-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 1774-1782.	0.2	0
4660	Crystal structures and hydrogen-bonding analysis of a series of solvated ammonium salts of molybdenum(II) chloride clusters. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 1705-1711.	0.2	1
4661	Underappreciated Chemical Interactions in Protein-Ligand Complexes. <i>Methods in Molecular Biology</i> , 2020, 2114, 75-86.	0.4	10
4662	Synergistic Effects of Hydration Sites in Protein Stability: A Theoretical Water Thermodynamics Approach. , 2020, , 187-212.		1

#	ARTICLE	IF	CITATIONS
4663	Crystal structures of (<i>E</i>)-5-(4-methylphenyl)-1-(pyridin-2-yl)pent-2-en-4-yn-1-one and [3,4-bis(phenylethynyl)cyclobutane-1,2-diyl]bis(pyridin-2-ylmethanone). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 192-196.	0.2	0
4664	Crystal structures and Hirshfeld surface analysis of <i>trans</i>-bis(thiocyanato- $\lambda^2$ -N)bis{2,4,6-trimethyl-N-[(pyridin-2-yl)methylidene]aniline- $\lambda^2$ -N <sub>2</sub> , <i>N</i>}. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 288-293.	0.2	0
4665	Dichloridobis[2-(pyridin-2-yl- $\lambda^2$ -N)-1<i>H</i>-benzimidazole- $\lambda^2$ -N <sup>3</sup>]nickel(II) monohydrate. IUCrData, 2020, 5, .	0.1	1
4666	Crystal structure, Hirshfeld surface analysis, interaction energy and DFT studies of (2<i>Z</i>)-2-(2,4-dichlorobenzylidene)-4-nonyl-3,4-dihydro-2<i>H</i>-1,4-benzothiazin-3-one. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 281-287.	0.2	1
4667	Crystal structure of a tripeptide biphenyl hybrid C<sub>50</sub>H<sub>56</sub>N<sub>6</sub>O<sub>10</sub>·0.5H<sub>2</sub>O. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 257-260.	0.2	1
4668	Research Data Reporting in Chemistry. , 2020, , .		1
4669	Crystallography Open Database (COD). , 2020, , 1863-1881.		8
4670	Bis{4-[(2-hydroxy-5-methoxy-3-nitrobenzylidene)amino]phenyl} ether. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 91-94.	0.2	0
4671	Crystal structures of chlorido[dihydroxybis(1-iminoethoxy)]arsanido- $\lambda^3$ -N<sub>2</sub>, <i>As</i>, <i>N</i>- $\lambda^2$ platinum(II) and of a polymorph of chlorido[dihydroxybis(1-iminopropoxy)arsanido- $\lambda^3$ -N<sub>2</sub>, <i>As</i>, <i>N</i>- $\lambda^2$ platinum(II). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 180-185.	0.2	0
4672	Crystal structure and Hirshfeld surface analysis of a copper(II) complex with ethylenediamine and non-coordinated benzoate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 111-114.	0.2	2
4673	Synthesis and crystal structure of 3-(adamantan-1-yl)-4-(2-bromo-4-fluorophenyl)-1<i>H</i>-1,2,4-triazole-5(4<i>H</i>)-thione. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 162-166.	0.2	2
4674	Poly[[tetradecakis( $\lambda^4$ -propionato)heptabarium] propionic acid monosolvate tetrahydrate]. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 264-269.	0.2	0
4675	Syntheses and crystal structures of 2,2,5-trimethyl-1,3-dioxane-5-carboxylic acid and 2,2,5-trimethyl-1,3-dioxane-5-carboxylic anhydride. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 86-90.	0.2	0
4676	Crystal structure and Hirshfeld surface analysis of 4-[(anthracen-9-yl)methyl]amino}benzoic acid. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 62-65.	0.2	2
4677	Structural characterization and Hirshfeld surface analysis of 2-iodo-4-(pentafluoro- $\lambda^6$ -sulfanyl)benzonitrile. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 231-234.	0.2	1
4678	Structural and theoretical study of four novel norcantharidine derivatives: two new cases of conditional isomorphism. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 75-86.	0.2	0
4679	A binuclear Cu<sup>II</sup>/Ca<sup>II</sup> thiocyanate complex with a Schiff base ligand derived from <i>o</i>-vanillin and ammonia. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 423-426.	0.2	2
4680	Crystal structure and Hirshfeld surface analysis of 4-allyl-2-methoxy-6-nitrophenol. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 461-465.	0.2	3



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4681	Crystal structure of the mixed methanol and ethanol solvate of bis{3,4,5-trimethoxy- <i>N</i> -[1-(pyridin-2-yl)ethylidene]benzohydrazidato}zinc(II). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 303-308.	0.2	0
4682	Crystal structure analysis of ethyl 3-(4-chlorophenyl)-1,6-dimethyl-4-methylsulfanyl-1 <i>H</i> -pyrazolo[3,4- <i>b</i> ]pyridine-5-carboxylate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 443-445.	0.2	2
4683	Synthesis, crystal structure, and thermal properties of poly[aqua( $\frac{1}{4}$ <sub>5</sub> -2,5-dicarboxybenzene-1,4-dicarboxylato)strontium]. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 354-359.	0.2	0
4684	Structural, Hirshfeld and DFT studies of conjugated <i>D</i> - <i>A</i> carbazole chalcone crystal. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 387-391.	0.2	5
4685	Crystal structure and Hirshfeld surface analysis of ( <i>E</i> )-3-(benzylideneamino)-5-phenylthiazolidin-2-iminium bromide. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 427-431.	0.2	0
4686	Syntheses and crystal structures of a new pyrazine dicarboxamide ligand, <i>N</i> - <sup>2</sup> , <i>N</i> - <sup>3</sup> -bis(quinolin-8-yl)pyrazine-2,3-dicarboxamide, and of a copper perchlorate binuclear complex. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 332-338.	0.2	0
4687	Crystal structure of a two-dimensional metal-organic framework assembled from lithium(I) and $\beta$ -cyclodextrin. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 349-353.	0.2	3
4688	Crystal structures and Hirshfeld surface analyses of two new tetrakis-substituted pyrazines and a degradation product. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 404-409.	0.2	1
4689	Crystal structure and Hirshfeld surface analysis of the methanol solvate of sclareol, a labdane-type diterpenoid. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 294-297.	0.2	1
4690	Crystal structure, Hirshfeld surface analysis and DFT studies of 1-[( <i>r</i> )-2, ( <i>c</i> )-6-diphenyl- <i>t</i> -3-(propan-2-yl)piperidin-1-yl]ethan-1-one. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 377-381.	0.2	0
4691	Crystal structure of poly[( $\frac{1}{4}$ <sub>3</sub> -4-amino-1,2,5-oxadiazole-3-hydroxamato)thallium(I)]. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 328-331.	0.2	0
4692	Interactions in flavanone and chalcone derivatives: Hirshfeld surface analysis, energy frameworks and global reactivity descriptors. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 212-224.	0.2	2
4693	Influence of fluorine substitution on the molecular conformation of 3- <i>deoxy</i> -3- <i>fluoro</i> -5-methyluridine. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 346-352.	0.2	0
4694	Crystal structure of ( <i>R</i> )-( <i>S</i> )-2-hydroxy-4-(methylsulfanyl)butanoic acid. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 562-566.	0.2	1
4695	Crystal structure of a new phenyl(morpholino)methanethione derivative: 4-[(morpholin-4-yl)carbothioyl]benzoic acid. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 581-584.	0.2	1
4696	Synthesis, structural characterization, and luminescence properties of heteroleptic bismuth-organic compounds. CrystEngComm, 2021, 23, 8183-8197.	1.3	6
4697	Poli-en isomorfisme in halogeengesubstitueerde 4-(fenielamino)pent-3-en-2-oon verbindings. South African Journal of Science and Technology, 2020, 38, 143-152.	0.1	0
4698	Silver(I) nitrate two-dimensional coordination polymers of two new pyrazinethiophane ligands: 5,7-dihydro-1 <i>H</i> ,3 <i>H</i> -dithieno[3,4- <i>b</i> ]:3,4,4'- <i>e</i> ]pyrazine and 3,4,8,10,11,13-hexahydro-1 <i>H</i> ,6 <i>H</i> -bis([1,4]dithiocino)[6,7- <i>b</i> :6,7'- <i>e</i> ]pyrazine. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 539-546.	0.2	4

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4699	Unexpected formation of a co-crystal containing the chalcone (<i>E</i>)-1-(5-chlorothiophen-2-yl)-3-(3-methylthiophen-2-yl)prop-2-en-1-one and the ketoâ€“enol tautomer (<i>Z</i>)-1-(5-chlorothiophen-2-yl)-3-(3-methylthiophen-2-yl)prop-1-en-1-ol. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 477-480.	0.2	3
4700	Crystal structure of (4-chlorophenyl)(4-methylpiperidin-1-yl)methanone. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 534-538.	0.2	1
4701	Poly[( $\frac{1}{4}$ -5,7-dihydro-1 <i>H</i> ,3 <i>H</i> -dithieno[3,4- <i>b</i> :3â€²,4â€²- <i>e</i> ]pyrazine- $\frac{1}{2}$ ) Tj ETQq0 copper(I) coordination polymer. IUCrData, 2020, 5, .	0.1	0
4702	Intramolecular 1,5-S...N $\pi$ -hole interaction in (<i>E</i>)- <i>N</i> -(pyridin-4-ylmethylidene)thiophene-2-carbohydrazide. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 557-561.	0.2	5
4703	Crystal structure and Hirshfeld surface analysis of 2-amino-3-hydroxypyridin-1-ium 6-methyl-2,2,4-trioxo-2 <i>H</i> ,4 <i>H</i> -1,2,3-oxathiazin-3-ide. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 572-575.	0.2	0
4704	2-amino-5-carboxyanilinium cation: C <sub>7</sub> H <sub>9</sub> N <sub>2</sub> O <sub>2</sub> + Cl <sup>-</sup> , C <sub>7</sub> H <sub>9</sub> N <sub>2</sub> O <sub>2</sub> + Br <sup>-</sup> and C <sub>7</sub> H <sub>9</sub> N <sub>2</sub> O <sub>2</sub> + NO <sub>3</sub> <sup>-</sup> . Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 637-641.	0.2	1
4705	Synthesis, crystal structure and Hirshfeld and thermal analysis of bis[benzyl 2-(heptan-4-ylidene)hydrazine-1-carboxylate] <sub>2</sub> nickel(II). Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 637-641.	0.2	0
4706	Synthesis and structure of ethyl 2-[(4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)sulfanyl]acetate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 668-672.	0.2	1
4707	Structure of a pushâ€“pull olefin prepared by ynamine hydroboration with a borandiol ester. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 710-714.	0.2	0
4708	Crystal structure and Hirshfeld surface analysis of 4-[(anthracen-9-yl)methyl]amino}benzoic acid dimethylformamide monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 728-731.	0.2	0
4709	Crystal structure and Hirshfeld surface analysis of 2-phenyl-1 <i>H</i> -phenanthro[9,10- <i>d</i> ]imidazol-3-ium benzoate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 724-727.	0.2	1
4710	Crystal structure, Hirshfeld surface analysis and interaction energy, DFT and antibacterial activity studies of ethyl 2-[( <i>Z</i> )-2-(2-chlorobenzylidene)-3-oxo-3,4-dihydro-2 <i>H</i> -1,4-benzothiazin-4-yl]acetate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 629-636.	0.2	1
4711	Crystal structure, Hirshfeld surface analysis and DFT studies of 6-bromo-3-(12-bromododecyl)-2-(4-nitrophenyl)-4 <i>H</i> -imidazo[4,5- <i>b</i> ]pyridine. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 677-682.	0.2	2
4712	Ditopic halogen bonding with bipyrimidines and activated pyrimidines. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 458-467.	0.2	5
4713	Synthesis and crystal structure of a pentacopper(II) 12-metallacrown-4: <i>cis</i> -diaquatetrakis(dimethylformamide- $\frac{1}{2}$ )manganese(II) tetrakis( $\frac{1}{4}$ -2,2-dioxidobenzene-1-carboximidate)pentacopper(II) dimethylformamide monosolvate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 747-751.	0.2	0
4714	Synthesis and crystal structure of a 6-chloronicotinate salt of a one-dimensional cationic nickel(II) coordination polymer with 4,4â€²-bipyridine. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 599-604.	0.2	2
4715	Chemical design of heterometallic carboxylate structures with Fe <sup>3+</sup> and Ag <sup>+</sup> ions as a rational synthetic approach. Mendeleev Communications, 2021, 31, 628-630.	0.6	3
4716	Impact of Nanoscale Morphology on Charge Carrier Delocalization and Mobility in an Organic Semiconductor. Advanced Materials, 2021, 33, e2104852.	11.1	9

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4717	A Molecular Compound for Highly Selective Purification of Ethylene. <i>Angewandte Chemie</i> , 2021, 133, 27390-27394.	1.6	4
4718	A Molecular Compound for Highly Selective Purification of Ethylene. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 27184-27188.	7.2	18
4719	Evaluation of Halogenopyridinium Cations as Halogen Bond Donors. <i>Crystal Growth and Design</i> , 2021, 21, 6889-6901.	1.4	14
4720	Crystal structures and Hirshfeld analysis of 4,6-dibromoindolenine and its quaternized salt. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 1203-1207.	0.2	0
4721	<i>N</i> - <i>tert</i> -Butyl-2-{2-[2-(4-chlorophenyl)-4-hydroxy-1-(5-methylisoxazol-3-yl)-5-oxo-2,5-dihydro-1 <i>H</i> -pyrrol-3-yl]- <i>N</i> -methanol monosolvate: single-crystal X-ray diffraction study and Hirshfeld surface analysis. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 1208-1212.	0.2	2
4722	Crystal structure of (+)-(1 <i>S</i> ,5 <i>S</i> ,6 <i>S</i> ,7 <i>S</i> ,10 <i>S</i> ,11 <i>S</i> ,16 <i>S</i> )-16-hydroxy-7-(methoxymethoxy)-1 <i>H</i> ,2 <i>H</i> ,15,18,18-tetramethyl-1 <i>H</i> -benzoate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 1234-1238.		
4723	Crystal structure and Hirshfeld surface analysis of 2-[[ <i>E</i> -(3-cyclobutyl-1 <i>H</i> -1,2,4-triazol-5-yl)imino]methyl]phenol. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 1267-1271.	0.2	5
4724	Pb <sup>II</sup> Oxo Interactions in Uranyl Hybrid Materials: A Combined Experimental and Computational Analysis of Bonding and Spectroscopic Properties. <i>Inorganic Chemistry</i> , 2021, 60, 17186-17200.	1.9	8
4725	Salts of 4-[(benzylamino)carbonyl]-1-methylpyridinium and iodide anions with different cation:iodine stoichiometric ratios. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 1219-1223.	0.2	0
4726	Synthesis and crystal structure of racemic ( <i>R</i> *, <i>R</i> *)-2,2- $\epsilon^2$ -(1,4-phenylene)bis(3-phenyl-2,3,5,6-tetrahydro-4 <i>H</i> -1,3-thiazin-4-one). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 1263-1266.	0.2	0
4727	The complex build algorithm to set up starting structures of lanthanoid complexes with stereochemical control for molecular modeling. <i>Scientific Reports</i> , 2021, 11, 21493.	1.6	2
4728	A homochiral coordination polymer of cobalt(II) and <i>L</i> -serine. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 764-769.	0.2	1
4729	Diversity of <i>N</i> -triphenylacetyl- <i>L</i> -tyrosine solvates with halogenated solvents. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 745-756.	0.2	0
4730	A bis-chelate <i>o</i> -vanillin-2-ethanolamine copper(II) complex bearing both imine and amine forms of the ligand. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 1272-1275.	0.2	1
4731	Crystal structures of the gold NHC complex bis(4-bromo-1,3-diethylimidazol-2-ylidene)gold(I) iodide and its 1:1 adduct with <i>trans</i> -bis(4-bromo-1,3-diethyl-imidazol-2-ylidene)diiodidogold(III) iodide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 1249-1252.	0.2	0
4732	Two metal-organic frameworks based on Sr <sup>2+</sup> and 1,2,4,5-tetrakis(4-carboxyphenyl)benzene linkers. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 1243-1248.	0.2	1
4733	Charge Assisted Hydrogen Bonded Assemblies and Unconventional O <sup>TM</sup> -O <sup>TM</sup> Dichalcogen Bonding Interactions in Pyrazole-Based Isostructural Ni(II) and Mn(II) Compounds involving Anthraquinone Disulfonate: Antiproliferative Evaluation and Theoretical Studies. <i>Journal of Molecular Structure</i> , 2021, 1250, 131883.	1.8	6
4734	Tris[triphenylantimony(V)]hexa( $\frac{1}{4}$ -oxido)tellurium(VI): a molecular complex with six Te <sup>VI</sup> -Sb bridges. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 1229-1233.	0.2	1

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4735	Crystal structure and self-assembly on graphite of a pyrazolo[1,5- <i>c</i> ]pyrimidine derivative. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 757-763.	0.2	0
4736	Deep Learning and Computational Chemistry. <i>Methods in Molecular Biology</i> , 2022, 2390, 125-151.	0.4	3
4737	Nonsteroidal Anti-Inflammatory Drugsâ€™ 1-Phenylethylamine Diastereomeric Salts: A Systematic Solid-State Investigation. <i>Crystal Growth and Design</i> , 2021, 21, 6947-6960.	1.4	7
4738	A Universal Force Field for Materials, Periodic GFN-FF: Implementation and Examination. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7827-7849.	2.3	10
4739	Crystal structure of bis(tetramethylthiourea- <i>S</i> )bis(thiocyanato- <i>N</i> )cobalt(II). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1373-1377.	0.2	3
4740	Crystal and molecular structure of [Ni{2-H <sub>2</sub> NC(=O)C <sub>5</sub> H <sub>4</sub> N}(H <sub>2</sub> O) <sub>2</sub> ][Ni{2,6-(O <sub>1</sub> )}] DFT studies on hydrogen bonding energies in the crystal. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2020, 76, 591-603.	0.5	1
4741	Structural characterization of the derivatives of bis{[2,6-(dimethylamino)methyl]phenyl} selenide with palladium(II) and mercury(II). <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 828-835.	0.2	0
4742	Caesium propanoate monohydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1307-1310.	0.2	2
4743	Crystal structure of 2,3-dimethoxy- <i>meso</i> -tetrakis(pentafluorophenyl)morpholinochlorin methylene chloride 0.44-solvate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1222-1228.	0.2	0
4744	Crystal structure analysis of ethyl 6-(4-methoxyphenyl)-1-methyl-4-methylsulfanyl-3-phenyl-1 <i>H</i> -pyrazolo[3,4- <i>b</i> ]pyridine-5-carboxylate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1209-1212.	0.2	1
4745	Crystal structures of two dysprosiumâ€™aluminiumâ€™sodium [3.3.1] metallacryptates that form two-dimensional sheets. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1378-1390.	0.2	3
4746	Crystal structure and Hirshfeld surface analysis of 2,6-diiodo-4-nitrotoluene and 2,4,6-tribromotoluene. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1391-1397.	0.2	0
4747	Syntheses and crystal structures of the anhydride 4-oxatetracyclo[5.3.2.0 <sup>2,6</sup> .0 <sup>8,10</sup> ]dodec-11-ene-3,5-dione and the related imide 4-(4-bromophenyl)-4-azatetracyclo[5.3.2.0 <sup>2,6</sup> .0 <sup>8,10</sup> ]dodec-11-ene-3,5-dione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1311-1315.	0.2	0
4748	Azetidin-2-ones: structures of antimitotic compounds based on the 1-(3,4,5-trimethoxyphenyl)azetidin-2-one core. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1187-1194.	0.2	1
4749	Synthesis, crystal structure at 219â€™.K and Hirshfeld surface analyses of 1,4,6-trimethylquinoxaline-2,3(1 <i>H</i> ,4 <i>H</i> )-dione monohydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1296-1301.	0.2	2
4750	From atoms to bonds, angles and torsions: molecular metrics from crystal space, and two <i>Excel</i> implementations. <i>Journal of Applied Crystallography</i> , 2020, 53, 1101-1107.	1.9	0
4751	Structural diversity in copper(I) iodide complexes with 6-thioxopiperidin-2-one, piperidine-2,6-dithione and isoindoline-1,3-dithione ligands. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1336-1344.	0.2	1
4752	Crystal structure, Hirshfeld surface analysis and DFT studies of 2-[(2-hydroxy-5-methylbenzylidene)amino]benzotrile. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1195-1200.	0.2	2





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4771	Two new polymorphic forms of combretastatin A-4, an antitumour agent. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 958-964.	0.2	0
4772	When solvent becomes reactant: a study of 6-aminothiocytosine derivatives. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 992-999.	0.2	0
4774	Crystal structures and phase transitions of imidazolium hypodiphosphates. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2020, 76, 939-947.	0.5	4
4775	Chlorido(4- $\kappa^2$ -chloro-2,2- $\kappa^2$ ,2- $\kappa^2$ -terpyridine- $\eta^3$ ) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 627 Td (<i>N</i> <i>S</i>). <i>IUCrData</i> , 2020, 5, .	0.1	0
4776	On the Hirshfeld surface for copper(II) atoms in different coordination environments. <i>Journal of Applied Crystallography</i> , 2020, 53, 1321-1333.	1.9	2
4778	Crystal structure of hyoscyamine sulfate monohydrate, (C <sub>17</sub> H <sub>24</sub> NO <sub>3</sub> ) <sub>2</sub> (SO <sub>4</sub> )(H <sub>2</sub> O). <i>Powder Diffraction</i> , 2020, 35, 286-292.	0.4	0
4779	Crystal structure of cephalexin monohydrate, C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub> S(H <sub>2</sub> O). <i>Powder Diffraction</i> , 2020, 35, 293-300.	0.4	3
4780	Powder X-ray diffraction of azelastine hydrochloride, C <sub>22</sub> H <sub>25</sub> ClN <sub>3</sub> O·Cl. <i>Powder Diffraction</i> , 2021, 36, 63-64.	0.4	0
4781	A cocrystal of L-ascorbic acid with picolinic acid: the role of O <sup>⋯</sup> H...O, N <sup>⋯</sup> H...O and C <sup>⋯</sup> H...O hydrogen bonds and L-ascorbic acid conformation in structure stabilization. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2020, 76, 967-978.	0.5	4
4782	Dibenzoate esters of cis-tetralin-2,3-diol as analogs of ( $\kappa^2$ )-epigallocatechin gallate: synthesis and crystal structure of anticancer drug candidates. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 1085-1095.	0.2	1
4783	Crystal structure of bis[ $\frac{1}{4}$ -N-( $\eta^2$ -prop-2-en-1-yl)piperidine-1-carbothioamide] <sup>2+</sup> S <sup>2-</sup> bis[(thiocyanato- $\eta^3$ -N)copper(I)]. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1712-1715.	0.2	0
4784	Synthesis and crystal structure of a heterobimetallic nickel <sup>II</sup> -manganese 12-metallacrown-4 methanol disolvate monohydrate compound. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 1720-1724.	0.2	0
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4790	Arginine off-kilter: guanidinium is not as planar as restraints denote. <i>Acta Crystallographica Section D: Structural Biology</i> , 2020, 76, 1159-1166.	1.1	7





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4935	Molecular modeling of indazole-3-carboxylic acid and its metal complexes (Zn, Ni, Co, Fe and Mn) as NO synthase inhibitors: DFT calculations, docking studies and molecular dynamics simulations. <i>Inorganic Chemistry Communication</i> , 2022, 135, 109120.	1.8	5
4936	Crystal structure of $\text{N,N,N,N-tetramethylethanediamine}$ . <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 36-39.	0.2	0

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4937	Bis( $\eta^5$ -cyclopentadienyl)(2-((2-methoxyphenyl)imino)methyl)phenolato- $\eta^3$ Tj ETQqO 0 0 rgBT /Overlock 10 Communications, 2022, 78, 44-46.	0.2	0
4938	Syntheses and crystal structures of 2-( <i>p</i> -tolyl)-1 <i>H</i> -perimidine hemihydrate and 1-methyl-2-( <i>p</i> -tolyl)-1 <i>H</i> -perimidine. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 169-172.	0.2	1
4939	Synthesis and structure of a new bulky bis(alkoxide) ligand on a terphenyl platform. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 92-96.	0.2	0
4940	Carboxamide carbonyl-ruthenium( $\eta^2$ ) complexes: detailed structural and mechanistic studies in the transfer hydrogenation of ketones. New Journal of Chemistry, 2022, 46, 3146-3155.	1.4	7
4941	Chemical crystallography by serial femtosecond X-ray diffraction. Nature, 2022, 601, 360-365.	13.7	33
4942	Synthesis, crystal structure and Hirshfeld surface analysis of 1-ferrocenylundecane-1,11-diol. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 149-153.	0.2	0
4943	Crystal structure of poly[[diaquatetra- $\eta^4$ -cyanido-platinum(II)iron(II)] methanol 4/3-solvate]: a three-dimensional Hofmann clathrate analogue. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 216-219.	0.2	1
4944	Crystal structure of hexasodium tetraserenolium paratungstate B decahydrate, $[\text{Na}_6\{(\text{CH}_2\text{OH})_2\text{CHNH}_3\}_4\text{W}_{12}\text{O}_{40}(\text{OH})_2]$ . Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 207-210.	0.2	0
4945	Crystal structure and Hirshfeld surface analysis of 5-acetyl-3-amino-6-methyl- <i>N</i> -phenyl-4-[( <i>E</i> )-2-phenylethenyl]thieno[2,3- <i>b</i> ]pyridine-2-carboxamide. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 225-230.	0.2	0
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4949	Synthesis and structural characterization of three new mixed ligand alkaline-earth metal picrates. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2022, 77, 211-219.	0.3	1
4950	Bildung und ReaktivitÄt eines Hydridosilikats $[\text{SiH}_6]^{2-}$ , koordiniert an einem durch einen Makrozyklus stabilisierten Strontiumkation. Angewandte Chemie, 0, , .	1.6	0
4951	Formation and Reactivity of a Hexahydridosilicate $[\text{SiH}_6]^{2-}$ Coordinated by a Macrocyclen-Supported Strontium Cation. Angewandte Chemie - International Edition, 2021, , .	7.2	6
4952	Crystal structure and Hirshfeld surface analysis of the hydrated 2:1 adduct of piperazine-1,4-dium 3,5-dinitro-2-oxidobenzoate and piperazine. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 198-202.	0.2	2
4953	$\text{Ni}^{\text{II}}$ molecular complex with a tetradentate aminoguanidine-derived Schiff base ligand: structural, spectroscopic and electrochemical studies and photoelectric response. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 173-178.	0.2	3
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4956	Crystal structure and Hirshfeld surface analysis of 3-(hydroxymethyl)-3-methyl-2,6-diphenylpiperidin-4-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 29-32.	0.2	2
4957	Crystal structure of diethanolbis(thiocyanato)bis(urotropine)cobalt(II) and tetraethanolbis(thiocyanato)cobalt(II)â€”urotropine (1/2). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 66-70.	0.2	1
4958	Synthesis, crystal structure and thermal properties of bis(1,3-dicyclohexylthiourea-Î²<i>S</i>)<i>bis</i>(isothiocyanato-Î²<i>N</i>)<i>cobalt</i>(II). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 71-75.	0.2	0
4959	Synthesis and crystal structures of three Schiff bases derived from 3-formylacetylacetone and<i>o</i>-,<i>m</i>- and<i>p</i>-aminobenzoic acid. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 54-59.	0.2	1
4960	Crystal structure and molecular docking study of diethyl 2,2â€”-({[(1<i>E</i>,<i>1â€”</i>)-hydrazine-1,2-diylidene]bis(methanylylidene)]bis(4,1-phenylene)}bis(oxy))diacetate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 88-91.		1
4961	Synthesis, crystal structure and Hirshfeld surface analysis of 2-(perfluorophenyl)acetamide in comparison with some related compounds. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 80-83.	0.2	5
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4964	Ultrahard magnetism from mixed-valence dilanthanide complexes with metal-metal bonding. <i>Science</i> , 2022, 375, 198-202.	6.0	246
4965	Reactive Oxygen Species Production Is Responsible for Antineoplastic Activity of Osmium, Ruthenium, Iridium and Rhodium Half-Sandwich Type Complexes with Bidentate Glycosyl Heterocyclic Ligands in Various Cancer Cell Models. <i>International Journal of Molecular Sciences</i> , 2022, 23, 813.	1.8	13
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4967	Crystallographic characterization of three cathinone hydrochlorides new on the NPS market: 1-(4-methylphenyl)-2-(pyrrolidin-1-yl)hexan-1-one (4-MPHP), 4-methyl-1-phenyl-2-(pyrrolidin-1-yl)pentan-1-one (Î±-PiHP) and 2-(methylamino)-1-(4-methylphenyl)pentan-1-one (4-MPD). <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 56-62.	0.2	2
4968	A novel hydrogen-bonding<i>N</i>-oxideâ€”sulfonamideâ€”nitro Nâ€”H...O synthon determining the architecture of benzenesulfonamide cocrystals. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 7-13.	0.2	1
4969	Experimental and computational evidence for stabilising parallel, offset Î€[C(=O)N(H)NÎ€]â€”Î€(phenyl) interactions in acetohydrazide derivatives. <i>CrystEngComm</i> , 2022, 24, 962-974.	1.3	0
4970	Cynarine monohydrate from synchrotron powder X-ray diffraction data. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 101-106.	0.2	0
4971	Binding Interactions in Copper, Silver and Gold Î€Complexes. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	15
4972	Synthesis and crystal structures of D-annulated pentacyclic steroids: looking within and beyond AR signalling in prostate cancer.. <i>CrystEngComm</i> , 0, , .	1.3	1



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4975	Relationship between the Crystal Structure and Tuberculostatic Activity of Some 2-Amidinothiosemicarbazone Derivatives of Pyridine. <i>Materials</i> , 2022, 15, 349.	1.3	1
4976	2.2.2-Cryptand complexes of neptunium(III) and plutonium(III). <i>Chemical Communications</i> , 2022, 58, 997-1000.	2.2	8
4977	The apparently unreactive substrate facilitates the electron transfer for dioxygen activation in Rieske dioxygenases. <i>Chemistry - A European Journal</i> , 2022, , .	1.7	6
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4979	3D QSAR and pharmacophore studies on inhibitors of insulin like growth factor 1 receptor (IGF-1R) and insulin receptor (IR) as potential anti-cancer agents. <i>Current Research in Chemical Biology</i> , 2022, 2, 100019.	1.4	2
4980	Crystal structure, Hirshfeld surface analysis and DFT study of 2,2-bis(1-phenylethyl)bis(azanylylidene))bis(3,6-bis(phenylthio)pyridine-2,5-dithiolene). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 1-7.	0.2	0
4981	An orthorhombic polymorph of 2-(1,3,5-dithiazinan-5-yl)ethanol or MEA-dithiazine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 191-197.	0.2	0
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4983	Crystal structure and Hirshfeld surface analysis of (S)-N-methyl-1-phenylethan-1-aminium chloride. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 130-134.	0.2	0
4984	4-[(Benzylamino)carbonyl]-1-methylpyridinium halogenide salts: X-ray diffraction study and Hirshfeld surface analysis. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 114-119.	0.2	0
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4992	Coordination complexes featuring bidentate $\hat{\text{N}}$ , $\hat{\text{I}}$ -8-iodoquinoline. <i>Journal of Coordination Chemistry</i> , 2021, 74, 3170-3181.	0.8	0
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4994	Electrochemically controlled cocrystallisation of caffeine:1-hydroxy-2-naphthoic acid. <i>CrystEngComm</i> , 2021, 24, 48-51.	1.3	8
4995	Synthesis and structural characterization of thallium and cadmium carbatrane compounds, [ $\text{http://www.w3.org/1998/Math/MathML}$ altimg="si1.svg"] <sup>2</sup> and [ $\text{http://www.w3.org/1998/Math/MathML}$ altimg="si1.svg"] <sup>2</sup> . <i>Polyhedron</i> , 2022, 222, 115642.	1.0	2
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4997	Tetranuclear and trinuclear copper( $\hat{\text{sc}}$ ) pyrazolates as catalysts in copper mediated azide $\hat{\text{E}}$ alkyne cycloadditions (CuAAC). <i>Dalton Transactions</i> , 2021, 51, 375-383.	1.6	12
4998	The Mechanochemical Synthesis and Activation of Carbon $\hat{\text{R}}$ ich $\hat{\text{I}}$ Conjugated Materials. <i>Advanced Science</i> , 2022, 9, e2105497.	5.6	28
4999	High-Fidelity Mock Development for the Insensitive High Explosive TATB. <i>Crystals</i> , 2022, 12, 192.	1.0	1
5000	Crystal structure, DFT and Hirshfeld surface analysis of $\hat{\text{N}}$ -acetyl- $\hat{\text{t}}$ -3-methyl- $\hat{\text{r}}$ -2, $\hat{\text{c}}$ -6-diphenylpiperidine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 179-183.	0.2	0
5001	The molecular and crystal structures of 2-(3-hydroxypropyl)benzimidazole and its nitrate salt. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 211-215.	0.2	1
5002	A tetranuclear nickel(II) complex, [ $\text{Ni}_4$ ]( $\hat{\text{L}}$ ) <sub>4</sub> ( $\text{ClO}_4$ ) <sub>4</sub> · $\hat{\text{C}}$ <sub>2</sub> $\hat{\text{H}}$ <sub>3</sub> $\hat{\text{N}}$ <sub>2</sub> $\hat{\text{O}}$ <sub>2</sub> with an asymmetric $\text{Ni}_4\text{O}_4$ open-cubane-like core. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 98-102.	0.2	0
5003	Crystal structure from X-ray powder diffraction data, DFT-D calculation, Hirshfeld surface analysis, and energy frameworks of ( $\hat{\text{R}}$ )-trichlormethiazide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 140-148.	0.2	2
5004	Redetermination of the structure of 2-amino-8-thia-1,5-diazaspiro[4.5]dec-1-en-5-ium chloride monohydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 164-168.	0.2	2
5005	Bis[3-(anthracen-9-yl)pentane-2,4-dionato- $\hat{\text{I}}$ <sup>2</sup> ]( $\hat{\text{N}}$ )-dimethylformamide- $\hat{\text{I}}$ tris(pyrazol-1-yl- $\hat{\text{N}}$ ) Tj ETQq0 0 0 ggBT /Overlock 10 Tf Communications, 2022, 78, 103-107.	0.2	0
5006	Crystal structure of a trifluoromethyl benzoato quadruple-bonded dimolybdenum complex. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 154-158.	0.2	1
5007	Computational studies of the magneto-structural correlations in a manganese dimer with Jahn $\hat{\text{E}}$ Teller distortions. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	1.3	1
5008	Crystal structures and Hirshfeld surface analyses of bis(4,5-dihydrofuran-2-yl)dimethylsilane and (4,5-dihydrofuran-2-yl)(methyl)diphenylsilane. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 23-28.	0.2	1

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5009	Crystal structure of a three-dimensional neodymium(III) coordination polymer, [Nd <sub>2</sub> (H <sub>2</sub> O) <sub>6</sub> (glutarato)(SO <sub>4</sub> ) <sub>2</sub> ] <sub>n</sub> . Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 159-163.	0.2	1
5010	Synthesis, crystal structure and Hirshfeld surface analysis of dimethyl 3-(3-bromophenyl)-6-methyl-7-oxo-3,5,6,7-tetrahydropyrazolo[1,2- <i>a</i> ]pyrazole-1,2-dicarboxylate. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 125-129.	0.2	0
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5013	Crystal structures of three <i>N,N,N'</i> -trisubstituted thioureas for reactivity-controlled nanocrystal synthesis. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 184-190.	0.2	1
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5017	Poly[dipotassium [[1/4 <sub>6</sub> -2,2',2'',2'''-[[pyrazine-2,3,5,6-tetrayltetrakis(methylene)]tetrakis(sulfanediy)]tetracetato]disilver(1) 5.2-hydrate]. IUCrData, 2022, 7, .		
5018	Crystal structures of two dioxomolybdenum complexes stabilized by salan ligands featuring phenyl and cyclohexyl backbones. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 244-250.	0.2	1
5019	Novel three-dimensional coordination polymer of 2-(1,3,5-triaza-7-phosphoniatricyclo[3.3.1.1 <sup>3,7</sup> ]decan-7-yl)ethanoic acid with silver(I) tetrafluoroborate. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 251-254.	0.2	0
5020	Synthesis, structure characterization and properties of a new oxidovanadium(IV) coordination polymer incorporating bridging (MoO <sub>4</sub> ) <sup>2-</sup> and (Mo <sub>8</sub> O <sub>26</sub> ) <sup>4-</sup> ligands. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2022, 77, 245-252.	0.3	2
5021	MOF Synthesis Prediction Enabled by Automatic Data Mining and Machine Learning. Angewandte Chemie, 0, , .	1.6	1
5022	Anion-assisted Fe(III)-coordination supramolecular systems based on 2,6-diacetylpyridine dihydrazone. Polyhedron, 2022, 215, 115679.	1.0	2
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5030	Single-crystal structure analysis of non-deuterated triglycine sulfate by neutron diffraction at 20 and 298 K: a new disorder model for the 298 K structure. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 306-312.	0.2	0
5031	Crystal structures of N-[4-(trifluoromethyl)phenyl]benzamide and N-(4-methoxyphenyl)benzamide at 173 K: a study of the energetics of conformational changes due to crystal packing. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 297-305.	0.2	1
5032	Crystal structure of 1,1,2,2,4,4-hexaisopropylmagnesiumocene. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 287-290.	0.2	1
5033	Distorted zinc coordination polyhedra in bis(1-ethoxy-2-[(2-methoxyethyl)imino]methyl)propan-1-olato)zinc, a possible CVD precursor for zinc oxide thin films. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 317-321.	0.2	0
5034	Crystal structures of two Co(NCS) <sub>2</sub> urotropine coordination compounds with different Co coordinations. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 264-269.	0.2	0
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5036	Crystal structure and Hirshfeld surface analysis of 5-acetyl-2-amino-4-(4-bromophenyl)-6-oxo-1-phenyl-1,4,5,6-tetrahydropyridine-3-carbonitrile. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 291-296.	0.2	9
5037	Crystal structure of tris(4,7-diphenyl-1,10-phenanthroline- $\text{N}^2$ )cobalt(III) tris(hexafluorophosphate) monohydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 313-316.	0.2	0
5038	Evaluating Hydrogen Bonding in Organic Cocrystals Using Low-Frequency Raman Vibrational Spectroscopy and Quantum Mechanical Simulations. <i>Crystal Growth and Design</i> , 2022, 22, 1922-1932.	1.4	5
5039	Cytotoxicity of piano-stool ruthenium cyclopentadienyl complexes bearing different imidato ligands. <i>Applied Organometallic Chemistry</i> , 2022, 36, .	1.7	6
5040	Mirror-plane disorder in a nickel chloride Schiff base complex: a suitable case study for crystallographic instruction. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 137-140.	0.2	1
5041	Mononuclear Transition Metal Cymantrenecarboxylates as Precursors for Spinel-Type Manganites. <i>Molecules</i> , 2022, 27, 1082.	1.7	3
5042	Synthesis and crystal structure of poly[[di- $\frac{1}{4}$ -( $\text{C}_3$ )-tetrathioantimonato-tris[(cyclam)cobalt(II)]] acetonitrile disolvate dihydrate] (cyclam = 1,4,8,11-tetraazacyclotetradecane). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 270-274.	0.2	1
5043	2,5-Diketopiperazines via Intramolecular N-Alkylation of Ugi Adducts: A Contribution to the Synthesis, Density Functional Theory Study, X-ray Characterization, and Potential Herbicide Application. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 1799-1809.	2.4	4
5044	2,5-Diiodothiophene: A Versatile Halogen Bonding Synthons for Crystal Engineering. <i>Crystal Growth and Design</i> , 2022, 22, 1906-1913.	1.4	7

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5045	Synthesis, Physicochemical, Thermal and Antioxidative Properties of Zn(II) Coordination Compounds with Pyrazole-Type Ligand. <i>Inorganics</i> , 2022, 10, 20.	1.2	2
5046	Packing Preferences of Chalcones: A Model Conjugated Pharmaceutical Scaffold. <i>Crystal Growth and Design</i> , 2022, 22, 1801-1816.	1.4	6
5047	Synthesis and characterization of nano-sized magnesium 1,4-benzenedicarboxylate metal organic framework via electrochemical method. <i>Journal of Solid State Chemistry</i> , 2022, 309, 122970.	1.4	1
5048	Decoding the Structure of Non-Proteinogenic Amino Acids: The Rotational Spectrum of Jet-Cooled Laser-Ablated Thioproline. <i>Molecules</i> , 2021, 26, 7585.	1.7	3
5049	Heterobimetallic Three-Dimensional 4 <i>d</i>-4 <i>f</i>; Coordination Polymers Based on 5-methyl-1-(pyridin-4-ylmethyl)-1 <i>H</i>-1,2,3-triazole-3,4-dicarboxylate. <i>SSRN Electronic Journal</i> , 0, .	0.4	0
5050	Unusual {<math>HC</math>O}<math>_n</math>, <math>n = 1</math> or 2, synthons predominate in the molecular packing of one-dimensional coordination polymers, {<math>Cd</math>S<math>_2</math>P(OR)<math>_2</math>}<math>_2</math>(<math>LH</math>)<math>_2</math>}, for R = Me and Et, but are precluded when R = i-Pr; <math>LH</math> = <math>N</math>-bis(3-pyridylmethyl)oxalamide. <i>CrystEngComm</i> , 0, .	1.3	0
5051	The structural complexity of perovskites. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 9196-9202.	1.3	4
5052	Resolving alternative structure determinations of indapamide using <math>^{13}</math>C solid-state NMR. <i>Chemical Communications</i> , 2022, 58, 4767-4770.	2.2	2
5053	Three-dimensional electron diffraction: a powerful structural characterization technique for crystal engineering. <i>CrystEngComm</i> , 2022, 24, 2719-2728.	1.3	5
5054	Remarkable stability of a molecular ruthenium complex in PEM water electrolysis. <i>Chemical Science</i> , 2022, 13, 3748-3760.	3.7	11
5055	Benchmarks of the density functional tight-binding method for redox, protonation and electronic properties of quinones. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6742-6756.	1.3	0
5056	Enhancing chalcogen bonding by metal coordination. <i>Dalton Transactions</i> , 2022, . .	1.6	9
5057	Influence of substituents in aryl groups on the structure, thermal transitions and electrorheological properties of zinc bis(diarylphosphate) hybrid polymers. <i>Dalton Transactions</i> , 2022, . .	1.6	1
5058	A chiral binaphthyl-based coordination polymer as an enantioselective fluorescence sensor. <i>Chemical Communications</i> , 2022, 58, 4512-4515.	2.2	10
5059	Control of supramolecular chirality in co-crystals of achiral molecules <i>via</i> stacking interactions and hydrogen bonding. <i>CrystEngComm</i> , 2022, 24, 2591-2601.	1.3	4
5060	MAGNETIC ANOMALIES IN POLYMERIC CHAIN COMPLEXES Cu(hfac)<math>_2</math> WITH SPIN-LABELED DIALKYLPIRAZOLES. <i>Journal of Structural Chemistry</i> , 2022, 63, 87-99.	0.3	5
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5062	Structural diversity and magnetic properties of copper(<math>quinaldinate</math>) compounds with amino alcohols. <i>New Journal of Chemistry</i> , 2022, 46, 6899-6920.	1.4	3



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5064	Do 2-coordinate iodine( <i>scpi</i> ) and silver( <i>scpi</i> ) complexes form nucleophilic iodonium interactions (Nils) in solution?. Chemical Communications, 2022, 58, 4977-4980.	2.2	9
5065	Effect of substituents in novel bioactive tavorole derivatives on intermolecular interactions hierarchy. CrystEngComm, 0, , .	1.3	2
5066	Synthesis and computational aspects of Al( <i>scpii</i> ) and Ga( <i>scpii</i> ) dihalides based on an amidinate scaffold. Dalton Transactions, 2022, 51, 4898-4902.	1.6	2
5067	Novel cyclen-polyiodide complexes: a reappraisal of I–I covalent and secondary bond limits. Dalton Transactions, 2022, 51, 10728-10739.	1.6	4
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5069	Structural topologies involving energetically significant antiparallel I–I stacking and unconventional N(nitrile)–I(fumarate) contacts in dinuclear Zn( <i>scpii</i> ) and polymeric Mn( <i>scpii</i> ) compounds: antiproliferative evaluation and theoretical studies. New Journal of Chemistry, 2022, 46, 5296-5311.	1.4	7
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5071	A rare example of a double metamagnetic transition leading to 2D and 3D long-range order in the two-dimensional pyrazine- and azido-bridged cobalt( <i>scpii</i> ) compound [Co(pyz)(N <sub>3</sub> ) <sub>2</sub> ]. Dalton Transactions, 2022, 51, 5617-5623.	1.6	2
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5077	Recent advances in the applications of thorium-based metal–organic frameworks and molecular clusters. Dalton Transactions, 2022, 51, 7376-7389.	1.6	19
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5079	Static discrete disorder in the crystal structure of iododiflunisal: on the importance of hydrogen bond, halogen bond and I–I stacking interactions. CrystEngComm, 0, , .	1.3	3
5080	Fragmentation and transferability in Hirshfeld atom refinement. IUCr, 2022, 9, 298-315.	1.0	7

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5082	Structural Characterization of Multicomponent Crystals Formed from Diclofenac and Acridines. <i>Materials</i> , 2022, 15, 1518.	1.3	4
5083	Insight of the various <i>in silico</i> screening techniques developed for assortment of cocrystal formers and their thermodynamic characterization. <i>Drug Development and Industrial Pharmacy</i> , 2021, 47, 1523-1534.	0.9	4
5084	Emerging Landscape of Computational Modeling in Pharmaceutical Development. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1160-1171.	2.5	18
5085	Tuning Photophysical Properties by p-Functional Groups in Zn(II) and Cd(II) Complexes with Piperonylic Acid. <i>Molecules</i> , 2022, 27, 1365.	1.7	10
5086	Two New Organic Co-Crystals Based on Acetamidophenol Molecules. <i>Symmetry</i> , 2022, 14, 431.	1.1	1
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5088	Crystal structure and Hirshfeld surface analysis of 2-oxo-2-phenylethyl 3-nitroso-2-phenylimidazo[1,2- <i>a</i> ]pyridine-8-carboxylate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 322-325.	0.2	0
5089	A new bioactive cocrystal of coumarin-3-carboxylic acid and thiourea: detailed structural features and biological activity studies. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 192-200.	0.2	4
5090	Dynamic simulation of orientational disorder in organic crystals: methyl groups, trifluoromethyl groups and whole molecules. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2022, 78, 333-343.	0.5	4
5091	Synthesis, Crystal Structure, and Hirshfeld Surface Analysis of Hexachloroplatinate and Tetrachlorouranyl of 3-Carboxypyridinium-Halogen Bonds and $\pi$ -Interactions vs. Hydrogen Bonds. <i>Crystals</i> , 2022, 12, 271.	1.0	13
5092	Interaction of Docetaxel with Phosphatidylcholine Membranes: A Combined Experimental and Computational Study. <i>Journal of Membrane Biology</i> , 2022, 255, 277-291.	1.0	4
5093	Organic materials repurposing, a data set for theoretical predictions of new applications for existing compounds. <i>Scientific Data</i> , 2022, 9, 54.	2.4	16
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5095	The Phosphorus Bond, or the Phosphorus-Centered Pnictogen Bond: The Covalently Bound Phosphorus Atom in Molecular Entities and Crystals as a Pnictogen Bond Donor. <i>Molecules</i> , 2022, 27, 1487.	1.7	17
5096	Data-Driven Matching of Experimental Crystal Structures and Gas Adsorption Isotherms of Metal-Organic Frameworks. <i>Journal of Chemical &amp; Engineering Data</i> , 2022, 67, 1743-1756.	1.0	6
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5100	Intermolecular Interactions Drive the Unusual Co-Crystallization of Different Calix[4]arene Conformations. Crystals, 2022, 12, 250.	1.0	1
5101	Crystal structure and Hirshfeld surface analysis of 2-amino-4-(4-methoxyphenyl)-6-oxo-1-phenyl-1,4,5,6-tetrahydropyridine-3-carbonitrile. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 330-335.	0.2	0
5102	A first-order phase transition in Blatter's radical at high pressure. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 107-116.	0.5	2
5103	Ethyl 10-cyano-7-hydroxy-6-oxo-3-phenyl-8,9,10,10a-tetrahydro-6 <i>H</i> -benzo[ <i>c</i> ]chromene-10-carboxylate. IUCrData, 2022, 7, .	0.1	1
5104	New Insight into Dearomatization and Decarbonylation of Antitubercular 4 <i>H</i> -Benzo[ <i>e</i> ][1,3]thiazinones: Stable 5 <i>H</i> - and 7 <i>H</i> -Benzo[ <i>e</i> ][1,3]thiazines. 1.6 ChemMedChem, 2022, 17, e202200021.		3
5105	CRYSTAL STRUCTURE OF HETEROLIGAND ZINC(II) COMPLEXES WITH PHOSPHORYLATED THIOAMIDE AND DIIMINES. Journal of Structural Chemistry, 2022, 63, 272-279.	0.3	1
5106	Crystal structure of (7-[[bis(pyridin-2-ylmethyl)amino]sup>3</sup>) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 467 Td (<i>N</i>/i> Section E: Crystallographic Communications, 2022, 78, 326-329.	0.2	0
5107	Frustrated and Realized Hydrogen Bonding in 4-Hydroxy-3,5-di <i>tert</i> -butylphenylphosphine Derivatives. Crystal Growth and Design, 2022, 22, 2512-2533.	1.4	8
5108	Crystal structures and Hirshfeld surface analysis of 5-amino-1-(4-methoxyphenyl)pyrazole-4-carboxylic acid and 5-amino-3-(4-methoxyphenyl)isoxazole. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 336-339.	0.2	0
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5118	Synthesis and Structural Characterization of Pyridine-2,6-dicarboxamide and Furan-2,5-dicarboxamide Derivatives. Molecules, 2022, 27, 1819.	1.7	4
5119	Ambroxol: Insight into the Crystal Structure, Hirshfeld Surface Analysis and Computational Study. Polycyclic Aromatic Compounds, 2023, 43, 2599-2617.	1.4	12
5120	Crystal structure and Hirshfeld surface analysis of tris(acetohydrazide- $\hat{P}^{2+}$ ) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 Crystallographica Section E: Crystallographic Communications, 2022, 78, 354-358.	0.2	0
5121	Anticooperativity of Multiple Halogen Bonds and Its Effect on Stoichiometry of Cocrystals of Perfluorinated Iodobenzenes. Crystal Growth and Design, 2022, 22, 2644-2653.	1.4	14
5122	Experimental and theoretical study of novel amino- $\hat{C}$ -functionalized P(V) coordination compounds suggested as inhibitor of M <sup>Pro</sup> of SARS-CoV-2 by molecular docking study. Applied Organometallic Chemistry, 2022, 36, e6636.	1.7	4
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5126	Deep learning modeling strategy for material science: from natural materials to metamaterials. JPhys Materials, 2022, 5, 014003.	1.8	6
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5128	Crystal structure of <i>cis</i> -7,8-dihydroxy-5,10,15,20-tetraphenylchlorin and its zinc(II)-ethylenediamine complex. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 392-398.	0.2	1
5129	Crystal structure of ( <i>E</i> )-3-({6-[2-(4-chlorophenyl)ethenyl]-3-oxo-2,3-dihydropyridazin-4-yl}methyl)pyridin-1-ium chloride dihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 458-462.	0.2	1
5130	Crystal structures of anhydrous and hydrated ceftibuten. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 381-384.	0.2	0
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5136	Carbon-Centered Hydrogen Bonds in Proteins. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1998-2008.	2.5	17
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5138	Chiral Resolution of <i>RS</i> -Baclofen via a Novel Chiral Cocrystal of <i>R</i> -Baclofen and <i>L</i> -Mandelic Acid. <i>Crystal Growth and Design</i> , 2022, 22, 2441-2451.	1.4	3
5139	Crystal structure and Hirshfeld surface analysis of 7,7-dimethyl-2-phenyl-3,3a,4,6,7,8,9,9a-octahydro-1 <i>H</i> -benzo[ <i>f</i> ]isoindole-1,5(2 <i>H</i> )-dione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 373-376.	0.2	0
5140	Crystal structure, Hirshfeld surface analysis, interaction energy and DFT calculations and energy frameworks of methyl 6-chloro-1-methyl-2-oxo-1,2-dihydroquinoline-4-carboxylate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 425-432.	0.2	2
5141	Crystal structure of 2-(2,5-dimethoxyphenyl)benzo[ <i>d</i> ]thiazole. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 445-448.	0.2	3
5142	<i>catena</i> -Poly[[tetrakis(3,5-dimethyl-1 <i>H</i> -pyrazole- <i>N</i> ) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 472 Td (<sup>2</sup>)] Hirshfeld surface analysis of a Cu<sup>II</sup> coordination polymer. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 433-438.	0.2	1
5143	Bis(catecholato- <i>η</i> <sup>2</sup> - <i>O</i> , <i>O</i> )bis(dimethyl sulfoxide- <i>η</i> <sup>2</sup> - <i>O</i> )titanium(IV). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 385-391.	0.2	0
5144	Investigation of crystal structures, energetics and isostructurality in halogen-substituted phosphoramidates. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2022, 78, 179-194.	0.5	1
5145	Powder X-ray diffraction as a powerful tool to exploit in organic electronics: shedding light on the first <i>N</i> , <i>N</i> , <i>N</i> , <i>N</i> -trialkylindolocarbazole. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2022, 78, 253-260.	0.5	1
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5147	Tetranuclear copper(II) complex of 2-hydroxy- <i>N</i> , <i>N</i> -bis[1-(2-hydroxyphenyl)ethylidene]propane-1,3-diamine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 349-353.	0.2	2
5148	Crystal structure and Hirshfeld surface analysis of 5-(5-phenyl-1,2-oxazol-3-yl)-1,3,4-thiadiazol-2-amine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 453-457.	0.2	0
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5151	Influence of Noncovalent Interactions on the Magnetic Behavior of Three Isostructural Layered Manganese(II) Dicarboxylate-Based Coordination Polymers. <i>Crystal Growth and Design</i> , 2022, 22, 2534-2546.	1.4	6
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5153	The Nitrogen Bond, or the Nitrogen-Centered Pnictogen Bond: The Covalently Bound Nitrogen Atom in Molecular Entities and Crystals as a Pnictogen Bond Donor. <i>Compounds</i> , 2022, 2, 80-110.	1.0	20
5154	Data Mining for Terahertz Generation Crystals. <i>Advanced Materials</i> , 2022, 34, e2107900.	11.1	26
5155	Topology-guided roadmap for reticular chemistry of metal-organic polyhedra. <i>CheM</i> , 2022, 8, 617-631.	5.8	10
5156	Crystal structure and Hirshfeld surface analysis of dimethyl 3,3-bis-[[1 <i>E</i> ,2 <i>E</i> ]-ethane-1,2-diylidene]bis(azanylylidene)}bis(4-methylbenzoate). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 340-345.	0.2	11
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5159	Crystal structure of <i>N</i> -(1 <i>H</i> -indol-2-ylmethylidene)-4-methoxyaniline. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 449-452.	0.2	0
5160	3-(Benzo[ <i>d</i> ]thiazol-2-yl)-2 <i>H</i> -chromen-2-one. <i>IUCrData</i> , 2022, 7, .	0.1	4
5161	Organic-inorganic hybrid mixed-halide Zn <sup>II</sup> and Cd <sup>II</sup> tetrahalometallates with the 2-methylimidazo[1,5- <i>a</i> ]pyridinium cation. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 359-364.	0.2	2
5162	Structural study of bioisosteric derivatives of 5-(1 <i>H</i> -indol-3-yl)-benzotriazole and their ability to form chalcogen bonds. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 418-424.	0.2	0
5163	Embroidering Ionic Cocrystals with Polyiodide Threads: The Peculiar Outcome of the Mechanochemical Reaction between Alkali Iodides and Cyanuric Acid. <i>Crystal Growth and Design</i> , 2022, 22, 2759-2767.	1.4	2
5164	Crystal structure of tetrakis(1/4-4-benzyl-4 <i>H</i> -1,2,4-triazole-1 <sup>o</sup> ) <i>N</i> Tj ETQq1 1 0.784314 rgBT /Overlock 10 T 5 <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 399-403.	0.2	0
5165	Inclusion of Pentamidine in Carboxylated Pillar[5]arene: Late Sequential Crystallization and Diversity of Host-Guest Interactions. <i>Crystal Growth and Design</i> , 2022, 22, 2854-2862.	1.4	4
5166	Acid-based analogs of certain water tetramers: an examination of some crystal structures in the literature. <i>Structural Chemistry</i> , 0, , 1.	1.0	0
5167	Fluorogenic Detection of Sulfite in Water by Using Copper(II) Azacyclam Complexes. <i>Molecules</i> , 2022, 27, 1852.	1.7	4
5168	Competition between Hydrogen and Anagostic Bonds in Ruthenocene Phases under High Pressure. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5028-5035.	1.5	5
5169	Synthesis of [2+2] Schiff base macrocycles by a solvent templating strategy and halogen bonding directed assembly. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 0, , 1.	0.9	2
5170	The Torsion Library: Semiautomated Improvement of Torsion Rules with SMARTScompare. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1644-1653.	2.5	4

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5172	Ratiometric Thermometers Based on Rhodamine B and Fluorescein Dye-Incorporated (Nano) Cyclodextrin Metal-Organic Frameworks. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 14367-14379.	4.0	18
5173	Crystal structure of 2-(benzo[ <i>d</i> ]thiazol-2-yl)-3,3-bis(ethylsulfanyl)acrylonitrile. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 369-372.	0.2	5
5174	Crystal structure and Hirshfeld surface analysis of ( <i>E</i> )-1-[2,2-dibromo-1-(2-nitrophenyl)ethenyl]-2-(4-fluorophenyl)diazene. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 404-408.	0.2	6
5175	Crystal structure and Hirshfeld surface analysis of 2-(2-hydroxyphenyl)quinoline-6-sulfonamide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 409-413.	0.2	0
5176	(18-Crown-6)-bis(tetrahydrofuran)-potassium Anthracenide: The Salt of a Free Radical Anion Crystallizing as a Kryptoracemate. <i>Chemistry</i> , 2022, 4, 137-145.	0.9	0
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5180	Crystal structure of a second polymorph of germacrone, C <sub>15</sub> H <sub>22</sub> O. <i>Powder Diffraction</i> , 0, , 1-7.	0.4	0
5181	Amorphous Inclusion Complexes: Molecular Interactions of Hesperidin and Hesperetin with HP- $\beta$ -CD and Their Biological Effects. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4000.	1.8	21
5182	Not dark yet for strong light-matter coupling to accelerate singlet fission dynamics. <i>Cell Reports Physical Science</i> , 2022, 3, 100841.	2.8	16
5183	Crystal structure of novel [Ni(2aepy)(2ampy)Cl(H <sub>2</sub> O)]Cl·H <sub>2</sub> O complex comprising both 2-aminoethylpyridine (2aepy) and 2-aminomethylpyridine (2ampy) ligands within the coordination sphere and comparison of its thermal properties with analogous Ni(II) complexes with 2ampy and 2aepy ligands. <i>Polyhedron</i> , 2022, , 115835.	1.0	0
5184	Bis(oxotremorine) fumarate bis(fumaric acid). <i>IUCrData</i> , 2022, 7, .	0.1	0
5185	A new pseudopolymorph of berberine chloride: crystal structure and Hirshfeld surface analysis. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 468-472.	0.2	1
5186	Synthesis and crystal structure of <i>anti</i> -10-butyl-10,11,22,23-tetrahydro-9 <i>H</i> ,21 <i>H</i> -5,8:15,12-bis(metheno)[1,5,11]triazacyclohexadiazino[1,1 <i>b</i> ]- <i>a</i> ...		
5187	Crystal structure of 4-bromo- <i>N</i> -(propylcarbamoyl)benzenesulfonamide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 485-489.	0.2	0
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5191	Synthesis, crystal structure and photophysical properties of chlorido[( <i>E</i> )-3-hydroxy-2-methyl-6-(quinolin-8-yl diazenyl)phenolato]copper(II) monohydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 473-476.	0.2	0
5192	Azide-Alkyne Interactions: A Crucial Attractive Force for Their Preorganization for Topochemical Cycloaddition Reaction. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	11
5193	Crystal structure of di- $\frac{1}{4}$ -chlorido-bis{chlorido[( $\eta^5$ )-5,6-pinenebipyridine]cobalt(II)} aquadichlorido[( $\eta^5$ )-5,6-pinenebipyridine]cobalt(II). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 464-467.	0.2	0
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5196	Iron(II), cobalt(II), and nickel(II) complexes with 1,10-phenanthroline and 2,2'-bipyridyl and the macropolyhedral borane cluster [trans-B <sub>20</sub> H <sub>18</sub> ] <sup>2-</sup> as counterion. <i>Polyhedron</i> , 2022, 217, 115740.	1.0	8
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5198	A rare diiodo-L-tyrosine copper(II) complexes - Crystal and molecular structure of materials stabilized by weak interactions. <i>Polyhedron</i> , 2022, 219, 115780.	1.0	0
5199	New Pt(II) diiodido complexes containing bidentate 1,3,4-thiadiazole-based ligands: Synthesis, characterization, cytotoxicity. <i>Inorganica Chimica Acta</i> , 2022, 536, 120891.	1.2	5
5200	Dual emission from Mn(II) complexes with carbazolyl-substituted phosphoramides. <i>Inorganica Chimica Acta</i> , 2022, 536, 120896.	1.2	8
5201	Structure and properties of phases in the Cu <sub>2</sub> -XSe-Sb <sub>2</sub> Se <sub>3</sub> system. The Cu <sub>2</sub> -XSe-Sb <sub>2</sub> Se <sub>3</sub> phase diagram. <i>Journal of Alloys and Compounds</i> , 2022, 906, 164384.	2.8	7
5202	Magnesium-catalyzed stereoselective transformations - A survey through recent achievements. <i>Polyhedron</i> , 2022, 219, 115790.	1.0	6
5203	Praseodymium trivalent ion is an effective inhibitor of mitochondrial basic amino acids and carnitine/acylcarnitine carriers. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2022, 1863, 148557.	0.5	1
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5205	Anion- $\pi$ stacks of Lindqvist superoctahedra [Mo <sub>6</sub> O <sub>19</sub> ] <sup>2-</sup> supported by caffeinium and theophyllinium cations. <i>Inorganica Chimica Acta</i> , 2022, 537, 120945.	1.2	2
5206	Study on the synthesis, physicochemical, electrochemical properties, molecular structure and antifungal activities of the 4-pyrrolidinopyridine Mg(II) meso-tetratolylporphyrin complex. <i>Journal of Molecular Structure</i> , 2022, 1261, 132882.	1.8	3

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5208	Effective adsorption of metolachlor herbicide by MIL-53(Al) metal-organic framework: Optimization, validation and molecular docking simulation studies. <i>Environmental Nanotechnology, Monitoring and Management</i> , 2022, 18, 100663.	1.7	5
5209	Formation of Spirocyclic Quaternary Ammonium Salts of N-Benzyl-1,5-Dimethyl-3,7-Diazabicyclo[3.3.1]nonan-9-ol due to Its Interaction with Terminal Dibromoalkanes. <i>Doklady Chemistry</i> , 2021, 500, 192-198.	0.2	0
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5211	Ab initio study of the biogenic amino acids. <i>Journal of Molecular Modeling</i> , 2021, 27, 355.	0.8	1
5212	Studies of the Formation and Stability of Ezetimibe-Cyclodextrin Inclusion Complexes. <i>International Journal of Molecular Sciences</i> , 2022, 23, 455.	1.8	5
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5215	Cones with a three-fold symmetry constructed from three hydrogen bonded theophyllinium cations that coat [FeCl <sub>4</sub> ] <sup>−</sup> anions in the crystal structure of tris(theophyllinium) bis(tetrachloridoferrate(III)) chloride trihydrate, C <sub>21</sub> H <sub>33</sub> Cl <sub>9</sub> Fe <sub>2</sub> N <sub>12</sub> O <sub>9</sub> . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2022, 237, 121-124.	0.1	2
5216	pyKVFinder: an efficient and integrable Python package for biomolecular cavity detection and characterization in data science. <i>BMC Bioinformatics</i> , 2021, 22, 607.	1.2	11
5217	Synthesis, Crystal Structure, and Spectral Study of a Novel Indenoimidazole Carboxylic Acid Amide. <i>Russian Journal of Organic Chemistry</i> , 2021, 57, 2018-2023.	0.3	1
5218	Synthesis, Structures, and Properties of a Series of Isostructural Lanthanide- $\Theta$ -Thiopheneacrylate Complexes. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2022, 648, .	0.6	1
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5222	Solubility Enhancement of Antidiabetic Drugs Using a Co-Crystallization Approach. <i>ChemistryOpen</i> , 2021, 10, 1260-1268.	0.9	8
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5224	Elucidating structural patterns in hydrogen bond dense materials: a study of ammonium salts of (4-aminium-1-hydroxybutylidene)-1,1-bisphosphonic acid.. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 0, , .	0.6	1

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5235	The Crystal Structure Elucidation of a Tetr peptide Analog of Somatostatin DOTA-Phe-D-Trp-Lys-Thr-OMe. <i>Crystals</i> , 2022, 12, 12.	1.0	1
5236	Diversifying Databases of Metal Organic Frameworks for High-Throughput Computational Screening. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 61004-61014.	4.0	50
5237	Native Cyclodextrins as Complexation Agents for Pterostilbene: Complex Preparation and Characterization in Solution and in the Solid State. <i>Pharmaceutics</i> , 2022, 14, 8.	2.0	8
5238	Breathing Room: Restoring Free Rotation in a Schiff-Base Macrocyclic through Endoperoxide Formation. <i>Organic Letters</i> , 2021, 23, 9538-9542.	2.4	1
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5244	Heuristics and Uncertainty Quantification in Rational and Inverse Compound and Catalyst Design. , 2024, , 485-495.		0
5245	<i>Ab initio</i> neural network MD simulation of thermal decomposition of a high energy material CL-20/TNT. Physical Chemistry Chemical Physics, 2022, 24, 11801-11811.	1.3	13
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5250	9-Trifluoromethylxanthenediols: Synthesis and Supramolecular Motifs. ACS Omega, 2022, 7, 13520-13528.	1.6	0
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5252	Exploring Photoswitchable Properties of Two Nitro Nickel(II) Complexes with (<math>N</math>,<math>N</math>,<math>O</math>)-Donor Ligands and Their Copper(II) Analogues. Inorganic Chemistry, 2022, 61, 6624-6640.	1.9	5
5253	A molecular substitutional disorder case study suitable for instruction: <math>L_2Cr^{II}(THF)_2[(trimethylsilyl)methyl]Cr^{III}</math> (<math>L</math> is 2,5-bis{[(2,6-diisopropylphenyl)imino]methyl}pyrrol-1-ide). Acta Crystallographica Section C, Structural Chemistry, 2022, 78, 295-298.	0.2	0
5254	Metal Coordination Enhances Chalcogen Bonds: CSD Survey and Theoretical Calculations. International Journal of Molecular Sciences, 2022, 23, 4188.	1.8	13
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5257	Synthesis and characterization of the 'Japanese rice-ball'-shaped Molybdenum Blue <math>Na_4[Mo_2O_2(OH)_4(C_6H_4NO_2)_2]</math>. Acta Crystallographica Section C, Structural Chemistry, 2022, 78, 299-304.		
5258	GEOM, energy-annotated molecular conformations for property prediction and molecular generation. Scientific Data, 2022, 9, 185.	2.4	50
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5262	4-[(Benzylamino)carbonyl]-1-methylpyridinium bromide hemihydrate: X-ray diffraction study and Hirshfeld surface analysis. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 496-499.	0.2	0
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5275	Data-Driven Materials Innovation and Applications. <i>Advanced Materials</i> , 2022, 34, e2104113.	11.1	51
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5282	Anion-anion interaction within Ch(CH <sub>3</sub> ) <sub>3</sub> X <sub>4</sub> <sup>+</sup> (Ch = S, Se, Te; X = Cl,) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 742 Td</i>	1.3	3
5283	Topological motifs in dicyanamides of transition metals. <i>CrystEngComm</i> , 2022, 24, 4740-4747.	1.3	3
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5285	Engineering Plastic Phase Transitions via Solid Solutions: The Case of "Reordering Frustration" in Ionic Plastic Crystals of Hydroxyquinuclidinium Salts. <i>Molecular Systems Design and Engineering</i> , 0, , .	1.7	1
5286	Solid forms and $\Gamma^2$ -cyclodextrin complexation of turinabol. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 305-313.	0.2	2
5287	Try Another Crystal: Crystal-Dependent Disorder of Pentaphosphaferrocene within the Same Crystallization. <i>Crystal Growth and Design</i> , 0, , .	1.4	2
5288	Interaction of ferric ions with europium metal organic framework and application to mineral processing sensing. <i>Philosophical Magazine</i> , 0, , 1-16.	0.7	1
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5292	Cost and potential of metal-organic frameworks for hydrogen back-up power supply. <i>Nature Energy</i> , 2022, 7, 448-458.	19.8	28
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5294	Halogen-bonded zigzag molecular network based upon 1,2-diiodoperchlorobenzene and the photoproduct <i>1,3-bis(pyridin-4-yl)-2,4-diphenylcyclobutane</i> . <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 506-509.	0.2	1
5295	2-Hydroxyethylammonium [2-(2,6-dichloroanilino)phenyl]acetate monohydrate. <i>IUCrData</i> , 2022, 7, .	0.1	0
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5297	Crystal structure and Hirshfeld surface analysis of (<math>E</math>)-1-[2,2-dibromo-1-(4-nitrophenyl)ethenyl]-2-(4-fluorophenyl)diazene. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 530-535.	0.2	5
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5299	Structural characterization of sodium and potassium 3-nitrohydrogenphthalate coordination polymers. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2022, .	0.3	0
5300	Crystal structure and photoluminescent properties of a new Eu(III)-phthalate-acetate coordination polymer. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 536-539.	0.2	2
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5302	New Strategies for Direct Methane-to-Methanol Conversion from Active Learning Exploration of 16 Million Catalysts. <i>Jacs Au</i> , 2022, 2, 1200-1213.	3.6	23
5303	<math>CELLOPT</math>: improved unit-cell parameters for electron diffraction data of small-molecule crystals. <i>Journal of Applied Crystallography</i> , 2022, 55, 647-655.	1.9	1
5304	Crystal structure and Hirshfeld surface analysis of 1-( <i>tert</i> -butylamino)-3-mesitylpropan-2-ol hemihydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 525-529.	0.2	9
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5309	Crystal structure and Hirshfeld surface analysis of 5-amino-5-oxo-2-oxo-2,3-dihydro-1 <i>H</i> -spiro[imidazo[1,2- <i>a</i> ]pyridine-7,3-indoline]-6,8-dicarbonitrile dimethyl sulfoxide disolvate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 554-558.	0.2	12
5310	Crystal structures of six 4-(4-nitrophenyl)piperazin-1-ium salts. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 510-518.	0.2	5
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5313	Molecular Fates of Organometallic Mercury in Human Brain. <i>ACS Chemical Neuroscience</i> , 2022, 13, 1756-1768.	1.7	12
5314	Isolation and structural comparison of Ru <sup>II</sup> -dnp complexes [dnp = 2,6-bis(1,8-naphthyridin-2-yl)pyridine] with axially or equatorially coordinating NCS ligands. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 545-549.	0.2	0
5315	Crystal structures of dimetal terephthalate dihydroxides, <i>M</i> <sub>2</sub> (C <sub>8</sub> H <sub>4</sub> O <sub>4</sub> ) <sub>2</sub> (OH) <sub>2</sub> ( <i>M</i> = Co, Ni, Zn) from powder diffraction data and DFT calculations. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 584-589.	0.2	1
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5324	Dibenzothiazepine Based MCR Chemistry. <i>European Journal of Organic Chemistry</i> , 2022, 2022, .	1.2	4
5325	Crystal structure and Hirshfeld surface analysis of ( <i>E</i> )-3-benzylidene-4-oxopentanoic acid. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 563-567.	0.2	1

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5356	tetraqua-Î¼<sub>3</sub>-fluorido-dodecakis(Î¼<sub>2</sub>-trifluoroacetato)<i>octahedro</i>-hexaytterbate(III) tetrahydrate, [(NH<sub>4</sub>)<sub>2</sub>]â€”(H<sub>3</sub>O)<sub>x</sub> (x = 1/4), containing a hexanuclear ytterbium(III) carboxylate complex with fa. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 608-614.	0.2	0
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5361	Crystal structure and Hirshfeld surface analysis of 2,4,6-triaminopyrimidine-1,3-dium dinitrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 669-674.	0.2	3

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5375	Crystal structure and Hirshfeld analysis of (1a <i>S</i> ,3a <i>R</i> ,4a <i>S</i> ,5a <i>R</i> )-15-acetoxylinden-7(11),8-trieno-12,8-lactone. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 642-646.	0.2	0
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5564	Two isomers Ba <sub>5</sub> Mg <sub>4</sub> C <sub>54</sub> O <sub>48</sub> H <sub>114</sub> and Pb <sub>5</sub> Mg <sub>4</sub> C <sub>54</sub> O <sub>48</sub> H <sub>114</sub> . <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2022, .	0.4	0
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5571	Synthesis, X-ray diffraction study, analysis of intermolecular interactions and molecular docking of ethyl 1-(3-tosylquinolin-4-yl)piperidine-4-carboxylate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 890-896.	0.2	1
5572	Crystal structure of 4,4-(diazenediyl)dipyridinium nitrate perchlorate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 897-899.	0.2	0
5573	Poly[bis(1/4<sub>-N</sub>-dimethylformamide-2<sup>2</sup>)] Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 227 Td	0.1	0
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5604	Crystal structure of aminopentamide hydrogen sulfate, (C <sub>19</sub> H <sub>25</sub> N <sub>2</sub> O)(HSO <sub>4</sub> ). <i>Powder Diffraction</i> , 0, , 1-6.	0.4	0
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5710	Synthesis, crystal structure and Hirshfeld surface analysis of <i>tert</i> -butyl <i>N</i> -acetylcarbamate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 1072-1076.	0.2	0
5711	Syntheses and crystal structures of benzyl $\alpha$ -(2-hydroxybenzylidene)hydrazinecarboxylate and benzyl $\alpha$ -(5-bromo-2-hydroxybenzylidene)hydrazinecarboxylate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 1010-1015.	0.2	1
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5729	Synthesis, crystal structures, and Hirshfeld analysis of three hexahydroquinoline derivatives. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 1089-1096.	0.2	0
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5739	Crystal structure of imepitoin, $C_{13}H_{14}ClN_3O_2$ . <i>Powder Diffraction</i> , 0, , 1-5.	0.4	0
5740	Crystal structure of haloxon, $C_{14}H_{14}Cl_3O_6$ . <i>Powder Diffraction</i> , 0, , 1-5.	0.4	0
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5784	Synthesis, crystal structure and Hirshfeld surface analysis of <i>catena</i>-poly[[bis(semicarbazide- <sup>2+</sup> <i>N</i>, <i>O</i>)copper(II)]- <sup>1/4</sup> -sulfato- <sup>2+</sup> <i>O</i>:<i>O</i>â€]. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 1131-1134.	0.2	0
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6095	<i>In situ</i> ligand restraints from quantum-mechanical methods. <i>Acta Crystallographica Section D: Structural Biology</i> , 2023, 79, 100-110.	1.1	4
6096	Machine learning in computational NMR-aided structural elucidation. , 0, 2, .		5
6097	Crystal structure of oxfendazole, C <sub>15</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> S. <i>Powder Diffraction</i> , 2023, 38, 37-42.	0.4	0
6098	Dynamic structural and microstructural responses of a metal-organic framework type material to carbon dioxide under dual gas flow and supercritical conditions. <i>Journal of Applied Crystallography</i> , 2023, 56, 222-236.	1.9	2
6100	A Computational Experiment Introducing Undergraduates to Geometry Optimizations, Vibrational Frequencies, and Potential Energy Surfaces. <i>Journal of Chemical Education</i> , 2023, 100, 921-927.	1.1	3
6101	Discovery of a Potent and Orally Bioavailable Zwitterionic Series of Selective Estrogen Receptor Degradator-Antagonists. <i>Journal of Medicinal Chemistry</i> , 2023, 66, 2918-2945.	2.9	7
6102	Computational Investigation of Structure-Function Relationship in Fluorine-Functionalized MOFs for PFOA Capture from Water. <i>Journal of Physical Chemistry C</i> , 2023, 127, 3204-3216.	1.5	9
6103	Solid-state NMR Spectroscopy of Iodine(I) Complexes. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	3
6104	Space group distributions differ considerably among subsets of organic crystal compounds: the impact of metal content and residue number. <i>CrystEngComm</i> , 2023, 25, 1467-1470.	1.3	1
6105	A New Motif in Halogen Bonding: Cooperative Intermolecular Br...O, O...F, and F...F Associations in the Crystal Packing of Di(sulfonyl bromide) Perfluoroalkanes. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	0
6106	Improving the Accuracy of Small-Molecule Crystal Structures Solved from Powder X-Ray Diffraction Data by Using External Sources. <i>Helvetica Chimica Acta</i> , 2023, 106, .	1.0	0
6107	Heteronuclear Bimetallic Complexes with 3d and 4f Elements. <i>MolBank</i> , 2023, 2023, M1577.	0.2	0
6108	Synthesis of Ti Complexes Supported by an <i>ortho</i> -Terphenoxide Ligand and Their Applications in Alkyne Hydroamination Catalysis. <i>Organometallics</i> , 2023, 42, 1732-1739.	1.1	2
6109	Syntheses and crystal structures of bis(4-methylpyridine- $\text{N}$ )bis(selenocyanato- $\text{N}$ )zinc(II) and <i>catena</i> -poly[[bis(4-methylpyridine- $\text{N}$ )cadmium(II)]-di- $\frac{1}{4}$ -selenocyanato- $\text{N}$ ] <sub>2</sub> Se <sub>2</sub> Se $\text{N}$ ]. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 136-141.	0.2	0
6110	Complexation between the Antioxidant Pterostilbene and Derivatized Cyclodextrins in the Solid State and in Aqueous Solution. <i>Pharmaceuticals</i> , 2023, 16, 247.	1.7	1
6111	In Silico High-Throughput Design and Prediction of Structural and Electronic Properties of Low-Dimensional Metal-Organic Frameworks. <i>ACS Applied Materials &amp; Interfaces</i> , 2023, 15, 9494-9507.	4.0	6
6112	Synthesis, crystal structure and Hirshfeld surface analysis of di- $\frac{1}{4}$ -iodido-bis[(2,2-biquinoline- $\text{N}$ )] <sub>2</sub> Se $\text{N}$ copper(I)]. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 132-135.	0.2	1
6113	Structure and Microbiological Activity of 1H-benzo[d]imidazole Derivatives. <i>International Journal of Molecular Sciences</i> , 2023, 24, 3319.	1.8	0

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6116	A Rigid Linker for Site-Selective Coordination of Transition Metal Cations: Combining an Acetylacetone with a Caged Phosphine. <i>Inorganic Chemistry</i> , 2023, 62, 3178-3185.	1.9	4
6117	Structures of <i>S</i> -(pyridin-2-yl) 4-nitrobenzothioate, <i>S</i> -(pyridin-2-yl) 4-methylbenzothioate and <i>S</i> -(pyridin-2-yl) 4-methoxybenzothioate: building blocks for low-symmetry multifunctional tetrapyrroles. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 157-162.	0.2	0
6118	Crystal structure and Hirshfeld surface analysis of 1-[( <i>E</i> )-2-(3-nitrophenyl)diazen-1-yl]naphthalen-2-ol. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 142-145.	0.2	1
6119	Synthesis, crystal structure and Hirshfeld surface analysis of the orthorhombic polymorph of 4-bromo- <i>N</i> -(4-bromobenzylidene)aniline. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 146-150.	0.2	0
6120	Bis( <i>N,N</i> -diethyl-4-methyl-4-piperazine-1-carboxamide) tetrakis(isothiocyanato- $\lambda^5$ -cobalt(II)), a model compound for the blue color developed in the Scott test. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 163-166.	0.2	2
6121	Short-Range Atomic Topology of Ab Initio Generated Amorphous PdSi Alloys. <i>Advanced Theory and Simulations</i> , 2023, 6, .	1.3	1
6122	Syntheses and crystal structures of four 4-(4-nitrophenyl)piperazinium salts with hydrogen succinate, 4-aminobenzoate, 2-(4-chlorophenyl)acetate and 2,3,4,5,6-pentafluorobenzoate anions. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 151-156.	0.2	0
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6124	Reactivity of a model of B3P3-doped nanographene with up to three CO <sub>2</sub> molecules. <i>Scientific Reports</i> , 2023, 13, .	1.6	4
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6126	Two Crystal Forms of 4-Methyl-2,4-dinitrodiphenylamine: Polymorphism Governed by Conformational Flexibility of a Supramolecular Synthron. <i>Crystals</i> , 2023, 13, 296.	1.0	0
6127	A Combined in Silico and Structural Study Opens New Perspectives on Aliphatic Sulfonamides, a Still Poorly Investigated Class of CA Inhibitors. <i>Biology</i> , 2023, 12, 281.	1.3	2
6128	Nature of NMR Shifts in Paramagnetic Octahedral Ru(III) Complexes with Axial Pyridine-Based Ligands. <i>Inorganic Chemistry</i> , 2023, 62, 3381-3394.	1.9	1
6129	On the Subset of Intermolecular Contacts Generating a Molecular Crystal: Topological Features of Organic Minerals. <i>Crystallography Reports</i> , 2022, 67, 1133-1145.	0.1	3
6130	Heteroleptic Copper Complexes as Catalysts for the CuAAC Reaction: Counter-Ion Influence in Catalyst Efficiency. <i>Catalysts</i> , 2023, 13, 386.	1.6	2
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6132	( <i>E</i> )-1,1'-[1,2-Bis(4-chlorophenyl)ethane-1,2-diyl]bis(phenyldiazene) revisited: threefold configurational disorder of ( <i>S</i> ), ( <i>R</i> ) and ( <i>S</i> , <i>R</i> ) isomers, a detailed critique. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2023, 79, 77-82.	0.2	3
6133	2d, or Not 2d: An Almost Perfect Mock of Symmetry. <i>Symmetry</i> , 2023, 15, 508.	1.1	0
6134	Disorder in 2-bromoimidazolium hexafluorophosphate salts: the role of halogen bonds. <i>CrystEngComm</i> , 2023, 25, 1763-1774.	1.3	1
6135	Phosphite Bearing [(1/4-ADT) <sub>2</sub> Fe(CO) <sub>6</sub> ] (ADT = Azadithiolate) Moieties: A Tool for the Building of Multimetallic [FeFe]-Hydrogenase Mimics. <i>Organometallics</i> , 2023, 42, 316-326.	1.1	2
6136	Overview on Theoretical Simulations of Lithium-Ion Batteries and Their Application to Battery Separators. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	29
6137	Dibromomethyl- and bromomethyl- or bromo-substituted benzenes and naphthalenes: C <sup>+</sup> Br...Br interactions. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2023, 79, 83-93.	0.2	1
6138	Crystal Engineering of Conglomerates: Dilution of Racemate-Forming Fe(II) and Ni(II) Congeners into Conglomerate-Forming [Zn(bpy) <sub>3</sub> ](PF <sub>6</sub> ) <sub>2</sub> . <i>Chemistry</i> , 2023, 5, 255-268.	0.9	0
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6141	One-pot synthesis and crystal structure of diethyl 2,6-dimethyl-4-(1-(2-nitrophenyl)-1 <i>H</i> -1,2,3-triazol-4-yl)-1,4-dihydropyridine-3,5-dicarboxylate, C <sub>21</sub> H <sub>23</sub> N <sub>5</sub> O <sub>6</sub> . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2023, 238, 381-384.	0.1	1
6142	Crystal structures of 4-(2/3-methoxyphenoxy)phthalonitrile. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 172-176.	0.2	1
6143	Crystal structures of two 1,2,3,4-tetrahydronaphthalenes obtained during efforts towards the total synthesis of elisabethin A. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 177-181.	0.2	0
6144	( <i>E</i> )- <i>N</i> -Phenyl- <i>N</i> -(phenylcarbamoyl)-3-[propyl(trimethylsilyl)amino]acrylamide chloroform hemisolvate. <i>IUCrData</i> , 2023, 8, .	0.1	0
6145	Synthesis, crystal structure and thermal properties of di-1/4-iodido-bis[bis(2-chloropyrazine-1 <i>N</i> )copper(I)]. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 167-171.	0.2	1
6146	Synthesis, crystal structure and properties of bis(isoselenocyanato-1 <i>N</i> )tetrakis(4-methoxypyridine-1 <i>N</i> )cobalt(II). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 216-220.	0.2	0
6147	BODIPY-Perylene Charge Transfer Compounds; Sensitizers for Triplet-Triplet Annihilation Up-conversion. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	5
6148	Halogen-bonded co-crystal containing 1,3-diiodoperchlorobenzene and the photoproduct <i>rtct</i> -tetrakis(pyridin-4-yl)cyclobutane resulting in a zigzag topology. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 212-215.	0.2	0
6149	Crystal structure and Hirshfeld surface analysis of isopropyl 4-[2-fluoro-5-(trifluoromethyl)phenyl]-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 187-191.	0.2	4

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6150	Synthesis, analysis of molecular and crystal structures, estimation of intermolecular interactions and biological properties of 1-benzyl-6-fluoro-3-[5-(4-methylcyclohexyl)-1,2,4-oxadiazol-3-yl]-7-(piperidin-1-yl)quinolin-4-one. Acta Crystallographica Section E: Crystallographic Communications, 2023, 79, 192-200.	0.2	0
6151	Optimizing disordered crystal structures. Acta Crystallographica Section C, Structural Chemistry, 2023, 79, 69-70.	0.2	0
6152	The crystal structure of 4â€“(4,4,5,5â€“tetramethylâ€“1,3,2â€“dioxaborolanâ€“2â€“(yl)morpholine, C <sub>10</sub> H <sub>20</sub> BNO <sub>3</sub> . Zeitschrift Fur Kristallographie - New Crystal Structures, 2023, .	0.1	0
6153	Crystal structures of di-1/4-chlorido-bis({(E)-5-(ethylamino)-4-methyl-2-[(pyridin-2-yl)diazenyl]phenolato}copper(II)) and chloridobis(1,10-phenanthroline)copper(II) chloride tetrahydrate. Acta Crystallographica Section E: Crystallographic Communications, 2023, 79, 201-206.	0.2	0
6154	Computational Modeling of 4d and 5d Transition Metal Catalysts. , 2024, , 601-621.		0
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6157	Machine learning-inspired battery material innovation. Energy Advances, 2023, 2, 449-464.	1.4	4
6158	Progress in Predicting Ionic Cocystal Formation: The Case of Ammonium Nitrate. Chemistry - A European Journal, 2023, 29, .	1.7	2
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6160	Synthesis of ONOâ€“Ligated Tetrylenes Based on 2,6â€“bis(2â€“Hydroxyphenyl)pyridines: Influence of Ligand Sterics on the Structure of the Products. European Journal of Inorganic Chemistry, 2023, 26, .	1.0	3
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6163	Synthesis, crystal structure and Hirshfeld surface analysis of bis[4-(2-aminoethyl)morpholine- <sup>1</sup> â€“ <sup>2</sup> <i>N</i>, <i>N</i>â€“ <sup>2</sup> ]diaquanickel(II) dichloride. Acta Crystallographica Section E: Crystallographic Communications, 2023, 79, 226-230.	0.2	2
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6171	<i>CrystalMELA</i>: a new crystallographic machine learning platform for crystal system determination. <i>Journal of Applied Crystallography</i> , 2023, 56, 409-419.	1.9	2
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6173	Crystal structure and Hirshfeld surface analysis of 2,5-diimino-8a-methyl-4,9-bis(4-methylphenyl)-7-oxo-6-phenyl-decahydro-2<i>H</i>-3,8-methanopyrano[3,2- <i>c&lt;/i&gt;]pyridine-3,4a-dicarbonyl-1,10-dimethylformamide monosolvate. <i>Acta Crystallographica Section E: Crystallographic Communications</i>, 2023, 79, 254-258.</i>	0.2	0
6174	Synthesis, X-ray characterization and DFT calculations of a series of 3-substituted 4,5-dichloroisothiazoles. <i>CrystEngComm</i> , 2023, 25, 1976-1985.	1.3	0
6175	On the origin of the combinatorial complexity of the crystal structures with 0D, 1D, or 2D primary motifs. <i>CrystEngComm</i> , 2023, 25, 2144-2158.	1.3	5
6176	Substituent Effects in Tetrel Bonds Involving Aromatic Silane Derivatives: An ab initio Study. <i>Molecules</i> , 2023, 28, 2385.	1.7	0
6177	Effect of steric hindrance on the interfacial connection of MOF-on-MOF architectures. <i>Nanoscale Advances</i> , 2023, 5, 2111-2117.	2.2	2
6178	Crystal Engineering of Two Light and Pressure Responsive Physisorbents. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	5
6179	Crystal Engineering of Two Light and Pressure Responsive Physisorbents. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	0
6180	<i>rac</i>-1-(4- <i>tert&lt;/i&gt;-Butylphenyl)-5-ethyl-4-ferrocenyl-5-hydroxy-1&lt;i&gt;H&lt;/i&gt;-pyrrol-2(5&lt;i&gt;H&lt;/i&gt;)-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i>, 2023, 79, 264-266.</i>	0.2	0
6181	Crystal structure of [2-([2-(dimethylamino- <i>Î</i> <sup>o</sup> <i>N</i>ethyl])imino- <i>Î</i> <sup>o</sup> <i>N</i>methyl)phenolato- <i>Î</i> <sup>o</sup> <i>O</i>](1,10-phenanthroline- <i>Î</i> <sup>o</sup> <sub>2</sub> <sup>o</sup> ) Tj ETQd Communications. 2023, 79, 259-263.	0.2	1
6182	Characterization and isolation of an 18-crown-6 complex of potassium hydroxide prepared by milling: application to mechanochemical organic synthesis. <i>New Journal of Chemistry</i> , 2023, 47, 7466-7469.	1.4	2
6183	Syntheses and crystal structures of three novel oxalate coordination compounds: Rb<sub>2</sub>Co(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>Â·4H<sub>2</sub>O, Rb<sub>2</sub>CoCl<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>) and K<sub>2</sub>Li<sub>2</sub>Cu(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>Â·2H<sub>2</sub>O. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 267-271.	0.2	0
6184	The dubious origin of beryllium toxicity. <i>Structural Chemistry</i> , 2023, 34, 391-398.	1.0	8
6185	Experimental and computational studies of tautomerism pyridine carbonyl thiosemicarbazide derivatives. <i>Structural Chemistry</i> , 0, , .	1.0	2







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6223	Crystal structure of [ <i>t</i> -BuMgCl] <sub>2</sub> [MgCl <sub>2</sub> (Et <sub>2</sub> O) <sub>2</sub> ]. Acta Crystallographica Section E: Crystallographic Communications, 2023, 79, 341-344.	0.2	0
6224	Crystal structure of trimethyl({tris[(phenylsulfanyl)methyl]silyl}methoxy)silane and Hirshfeld surface analysis of 3-bromo-2,2-bis(bromomethyl)propan-1-ol. Acta Crystallographica Section E: Crystallographic Communications, 2023, 79, 323-327.	0.2	0
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6226	Synthesis and crystal structure of <i>N</i> -(5-acetyl-4-methylpyrimidin-2-yl)benzenesulfonamide. Acta Crystallographica Section E: Crystallographic Communications, 2023, 79, 331-334.	0.2	0
6227	Crystal structures of three homologues with increasing ring size: 2-methoxy-4-(thiophen-2-yl)-5,6,7,8-tetrahydroquinoline-3-carbonitrile, 2-methoxy-4-(thiophen-2-yl)-6,7,8,9-tetrahydro-5 <i>H</i> -cyclohepta[ <i>b</i> ]pyridine-3-carbonitrile and 2-methoxy-4-(thiophen-2-yl)-5,6,7,8,9,10-hexahydrocycloocta[ <i>b</i> ]pyridine-3-carbonitrile. Acta Crystallographica Section E: Crystallographic Communications, 2023, 79, 335-340.	0.2	0
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6230	Discovery of novel arylpiperazine-based DA/5-HT modulators as potential antipsychotic agents – Design, synthesis, structural studies and pharmacological profiling. European Journal of Medicinal Chemistry, 2023, 252, 115285.	2.6	1
6231	Sulfonamide derived Schiff base Mn (II), Co (II), and Ni (II) complexes: Crystal structures, density functional theory and Hirshfeld surface analysis. Applied Organometallic Chemistry, 2023, 37, .	1.7	13
6232	Tb <sub>2</sub> O@C <sub>2</sub> (1333)-C <sub>74</sub> : A Non-Isolated Pentagon Endohedral Fullerene Containing a Nearly Linear Tb“O”Tb Unit. Inorganic Chemistry, 2023, 62, 5114-5122.	1.9	3
6233	Crystal structure and Hirshfeld surface analysis of <i>N</i> -[amino(dimethylamino)methyl]carbamidoyl-3-bromobenzenesulfonamide. Acta Crystallographica Section E: Crystallographic Communications, 2023, 79, 367-372.	0.2	0
6234	3,3'-Bis(Phenylmethylene)bis(1-ethyl-3,4-dihydro-1 <i>H</i> -2,1-benzothiazine-2,2,4-trione): single-crystal X-ray diffraction study, quantum-chemical calculations and Hirshfeld surface analysis. Acta Crystallographica Section E: Crystallographic Communications, 2023, 79, 349-355.	0.2	0
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6239	Crystal structure and DFT calculations of Cp <sub>2</sub> NbH(SiIm <sub>2</sub> )(SiFM <sub>2</sub> ): an asymmetric bis(silyl) niobocene hydride complex. Acta Crystallographica Section C, Structural Chemistry, 2023, 79, 158-163.	0.2	0
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