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Supporting information for article:

**The Cambridge Structural Database in chemical education:
analysis of hydrogen bonded networks in salts of hexa-aqua metal
ions with organic counterions**

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Supporting information includes a spreadsheet file (Microsoft Excel xlsx format; pdf version included here) listing for each of the 134 selected crystal structures: CSD refcode, metal cation, anion, short description of the hydrogen-bond network, presence of cation-cation and anion-anion hydrogen bonds, cases where non-ionic functional groups belonging to anions are involved in hydrogen bonds with cations, isomorphous structures, polymorphs, space group, R-factor, useful remarks. Filtering and sorting on each of these columns allow the interested reader to select structure subsets for programming teaching activities.

REFCODE	HEXAQUA CATION	ORGANIC ANION	HYDROGEN BOND FRAMEWORK	HB AMONG CATIONS	HB AMONG ANIONS	NON ANIONIC GROUP HB TO CATION	ISOMORPH	POLYMORPH	SPACE GROUP	R FACTOR %	REMARKS
AJIDON	cobalt(ii)	bis(4-amino-3-methylbenzenesulfonate)	(001) interconnected layers	no	[010] zigzag chain	yes	AJIDON		P2 ₁ /n	2.75	
AJIDUT01	magnesium(ii)	bis(4-amino-3-methylbenzenesulfonate)	(001) interconnected layers	no	[010] zigzag chain	yes	AJIDON		P2 ₁ /n	2.50	
AJOTAX	iron(ii)	bis(4-chlorobenzenesulfonate)	(001) interdigitated layers	no	no	no			P2 ₁ /n	3.45	
AMIPAP	manganese(ii)	bis(3-carboxythiophene-2-carboxylate)	(100) stacked layers	no	no	no			P-1	4.91	
AQMEDA	magnesium(ii)	dihydrogen ethylenediaminetetraacetate	(100) interconnected layers	no	(100) layer	no			P2 ₁ /c	7.05	
AQOXIO	copper(ii)	2,3,5,6-tetrafluorobenzene-1,4-disulfonate	(001) interconnected layers	[100] chain	no	no			P-1	2.65	
ASUDIB	cobalt(ii)	benzene-1,4-dioxyacetate	(001) interconnected layers	[100] chain	no	no	ASUDIB		P-1	2.60	
ATUNAE	manganese(ii)	benzene-1,4-dioxyacetate	(001) interconnected layers	[100] chain	no	yes	ASUDIB		P-1	2.87	
BAVYOM	cobalt(ii)	bis(1-oxo-1-pyridine-4-carboxylate)	(100) interconnected layers	no	no	yes	BAVYOM		P2 ₁ /c	4.05	
BAVYOM02	cobalt(ii)	bis(1-oxo-1-pyridine-4-carboxylate)	(001) interconnected layers	no	no	yes	BAVYOM02		C2/m	2.35	
BAVYUS01	nickel(ii)	bis(1-oxo-1-pyridine-4-carboxylate)	(100) interconnected layers	no	no	yes	BAVYOM		P2 ₁ /c	3.78	
BEMWUM	manganese(ii)	bis(3-(4-methoxyphenyl)-1,2-dioxocyclobut-3-en-4-olate)	(001) interdigitated layers	no	no	no	BEMWUM		P2 ₁ /c	2.52	
BEMXAT	nickel(ii)	bis(3-(4-methoxyphenyl)-1,2-dioxocyclobut-3-en-4-olate)	(001) interdigitated layers	no	no	no	BEMWUM		P2 ₁ /c	7.59	
BENBIG01	zinc(ii)	bis(trifluoromethanesulfonate)	(001) stacked layers	no	no	no	BENBIG01		P-3m1	3.86	
BENSCU	copper(ii)	bis(benzenesulfonate)	(100) interdigitated layers	no	no	no	Isostructural		P-1	3.22	
BISCOX	cadmium(ii)	bis(camphor-10-sulfonate)	(001) stacked layers	no	no	no			P2 ₁	6.69	
BOGRIA	zinc(ii)	bis((phenylsulfonyl)methanesulfinate)	(010) stacked layers	(010) layer	no	yes			P2 ₁	3.15	
BUGFEO	cobalt(ii)	bis(N-phenylsalicylaldimine-5-sulfonate)	(001) interdigitated layers	no	no	no			C2/m	4.70	anion with intramolecular H-bond
BUVRAM	magnesium(ii)	bis((1,2,4-triazol-1-yl)acrylate)	(001) interconnected layers	no	no	yes			P-1	3.80	
CAGVOV03	cobalt(ii)	2,5-dicarboxylato-benzene-1,4-dicarboxylic acid	(100) interconnected layers	[001] zigzag chain	no	no	CAGVOV03		C2/c	4.40	anion with intramolecular H-bond
CIRVAA02	magnesium(ii)	bis(hydrogen maleate)	(100) interconnected layers	no	no	no			P2 ₁ /c	4.80	anion with intramolecular H-bond
CITDAK	zinc(ii)	bis(1-oxo-1-pyridine-4-carboxylate)	(100) interconnected layers	no	no	yes	BAVYOM		P2 ₁ /c	2.49	
CITDAK02	zinc(ii)	bis(1-oxo-1-pyridine-4-carboxylate)	(001) interconnected layers	no	no	yes	BAVYOM02		C2/m	4.81	
COCXIC	manganese(ii)	bis(1-(4-hydroxyphenyl)-1H-tetrazol-5-yl-thioacetate)	(001) interconnected layers	no	dimer	yes	COCXIC		P-1	3.30	
COCXOI	cobalt(ii)	bis(1-(4-hydroxyphenyl)-1H-tetrazol-5-yl-thioacetate)	(001) interconnected layers	no	dimer	yes	COCXIC		P-1	4.50	
COCXUO	nickel(ii)	bis(1-(4-hydroxyphenyl)-1H-tetrazol-5-yl-thioacetate)	(001) interconnected layers	no	dimer	yes	COCXIC		P-1	5.60	
COCYAV	zinc(ii)	bis(1-(4-hydroxyphenyl)-1H-tetrazol-5-yl-thioacetate)	(001) interconnected layers	no	dimer	yes	COCXIC		P-1	5.07	
COHDPH	cobalt(ii)	bis(hydrogenphthalate)	(010) stacked layers	[101] chain	[100] zigzag chain	no			P2 ₁ /c	2.92	
COHDPH01	cobalt(ii)	bis(hydrogenphthalate)	(100) stacked layers	no	no	no			C2/m	2.71	anion with intramolecular H-bond
COHDPH02	cobalt(ii)	bis(hydrogenphthalate)	(001) stacked layers	no	[100] zigzag chain	no			P2 ₁ /a	2.80	
COHSUP	manganese(ii)	bis(2,6-dichlorobenzoate)	(001) stacked layers	[100] chain	no	no			P2 ₁ /c	2.60	
CUPVEP	magnesium(ii)	bis(2-carbamoyl-4-nitrobenzoate)	(100) stacked layers	no	[001] zigzag chain	yes			P2 ₁ /c	2.46	
DEVTUW	magnesium(ii)	5,5'-bis(nitroimino)-1,1',5,5'-tetrahydro-3,3'-bi-1,2,4-triazol-4-ide	(001) interconnected layers	no	[110] chain	yes			P-1	4.81	
DILCIL	copper(ii)	bis(4-hydroxybenzenesulfonate)	(001) interconnected layers	no	no	yes			P2 ₁ /n	3.79	
DIRXUA	magnesium(ii)	bis(1-amino-1H-tetrazol-5-olate)	(001) interconnected layers	no	[100] chain	yes			P-1	2.73	
DIWLUS	zinc(ii)	bis(6-methyl-2-oxo-1,2-dihydropyridine-4-carboxylate)	(001) interconnected layers	no	dimer	yes			C2/c	2.77	
DOFXIG	magnesium(ii)	bis(3,5-dinitropyridin-4-one)	(100) interconnected layers	no	no	yes			P2 ₁ /c	3.18	
DUBYIJ	cobalt(ii)	2,2'-(1,3-propanediyl)bis(sulfanediy-1H-tetrazole-5,1-diyl)diacetate	(100) interconnected layers	no	no	yes			C2/c	4.50	
DURPIQ	cobalt(ii)	3,3'-dicarboxybiphenyl-4,4'-dicarboxylate	(001) interconnected layers	no	no	no	DURPIQ		P-1	1.88	anion with intramolecular H-bond
EQEHEO	nickel(ii)	3,3'-(1,4-phenylenebis(methyleneimino))dibenzoate	(100) interconnected layers	(100) layer	(100) layer	no			P2 ₁ /c	4.30	
FAFYIX	manganese(ii)	bis((E)-4-((4-(dimethylamino)phenyl)diazenyl)benzenesulfonate)	(001) interdigitated layers	no	no	no	FAFYIX		P2 ₁ /c	3.01	
FAWBEM	manganese(ii)	bis(trifluoromethanesulfonate)	(100) stacked layers	no	no	no	FAWBEM		C2/m	7.70	
FETHAO	magnesium(ii)	benzene-1,4-dioxyacetate	(001) interconnected layers	[100] chain	no	yes	ASUDIB		P-1	3.01	
FEYTIN	manganese(ii)	5,5'-(1,4-phenylene)ditetrazolate	[100] chains	[100] chain	no	no			P2 ₁ /n	5.98	
FINNUM	copper(ii)	bis(naphthalene-2-sulfonate)	(001) interdigitated layers	no	no	no	FINNUM		P2 ₁ /n	3.63	
FOGWUU	zinc(ii)	naphthalene-1,5-disulfonate	(100) interconnected layers	(100) layer	no	no	FOGWUU		P2 ₁ /c	7.31	
FONDOC01	nickel(ii)	bis(6-oxo-1,6-dihydropyridine-3-carboxylate)	(001) interconnected layers	no	no	yes			P-1	3.13	
GOLSUX	iron(ii)	2,5-dicarboxylato-benzene-1,4-dicarboxylic acid	(100) interconnected layers	[001] zigzag chain	no	no	CAGVOV03		C2/c	5.00	anion with intramolecular H-bond
HEFSAM	cobalt(ii)	bis(4-hydroxy-3-nitrobenzenesulfonate)	(010) interconnected layers	[001] chain	dimer	no			P-1	3.90	pillars connected through H-bonds
HEHSIW	manganese(ii)	pyrazine-3,6-dicarboxylato-2,5-dicarboxylic acid	(001) interconnected layers	[100] zigzag chain	no	yes			A2/n	2.20	
HETZUB	magnesium(ii)	bis(4-chloro-(E)-3-phenyl-2-propenoate)	(001) interconnected layers	(001) layer	no	no			P2 ₁ /n	2.87	
HIPZAI	cadmium(ii)	bis(1-(4-hydroxyphenyl)-1H-tetrazol-5-yl-thioacetate)	(001) interconnected layers	no	dimer	yes	COCXIC		P-1	3.60	
IRONIM	cobalt(ii)	naphthalene-1,5-disulfonate	(100) interconnected layers	(100) layer	no	no	FOGWUU		P2 ₁ /c	6.41	
JAXYUF	magnesium(ii)	bis(5-(4H-1,2,4-triazol-4-yl)tetrazol-2-ide)	(010) interconnected layers	no	no	yes			P2 ₁ /n	2.82	
JEYCEW	magnesium(ii)	tetrathiosquarate	(100) interconnected layers	[010] chain	no	no			C2/c	5.70	O-H...S interactions
JIKYAG	cobalt(ii)	bis(naphthalene-2-sulfonate)	(001) interdigitated layers	[010] chain	no	no	FINNUM		P2 ₁ /n	6.98	
KADFIG	copper(ii)	bis(3-(4-nitrophenyl)-2-phenylpropenoate)	(001) interdigitated layers	[100] chain	no	yes			P-1	3.45	
KOZXOP	magnesium(ii)	bis(3,4-dinitropyrazol-1-ide)	(001) interconnected layers	no	no	yes			P-1	4.54	
KURWOK	magnesium(ii)	bis(4-(3-ethoxy-2-hydroxybenzylideneamino)-3-methylbenzenesulfonate)	(100) interdigitated layers	no	no	no			C2/c	2.77	anion with intramolecular H-bond
LIJSOM	nickel(ii)	bis(D-camphor-10-sulfonate)	(001) stacked layers	no	no	no	LIJSOM		P2 ₁	8.30	
LIYYAT	cobalt(ii)	bis(4-methylbenzenesulfonate)	(001) interdigitated layers	no	no	no	LIYYAT		P2 ₁ /n	5.14	
LUMVAQ	nickel(ii)	naphthalene-1,5-disulfonate	(100) interconnected layers	(100) layer	no	no	FOGWUU		P2 ₁ /c	2.50	
LUZZUC	magnesium(ii)	bis(2-(thiosemicarbazonomethyl)benzoate)	(100) interconnected layers	no	[010] zigzag chain	yes			P2 ₁ /c	4.00	N-H...S interactions
MEHKUG	manganese(ii)	bis(2-(carboxylatomethylsulfanyl)pyridine N-oxide)	(001) interconnected layers	no	no	yes			P2 ₁ /c	2.59	
MGNTSP	magnesium(ii)	bis(p-nitrosophenolate)	(100) interconnected layers	no	no	yes			P2 ₁ /c	4.69	
MINKOJ	magnesium(ii)	bis(o-benzenedisulfonimide)	(001) interdigitated layers	no	no	no			P-1	3.80	
MODFAN	magnesium(ii)	bis(D-camphor-10-sulfonate)	(001) stacked layers	no	no	no	LIJSOM		P2 ₁	6.80	
NERGEY	cobalt(ii)	bis(adamantane-1-sulfonate)	(001) stacked layers	no	no	no			C2/m	3.60	
NUHROY	magnesium(ii)	bis(1-oxopyridinium-2-sulfanylpropionate)	(001) interconnected layers	no	no	yes	NUHROY		P-1	4.58	
NUHRUE	nickel(ii)	bis(1-oxopyridinium-2-sulfanylpropionate)	(001) interconnected layers	no	no	yes	NUHROY		P-1	2.90	
NUHSAL	zinc(ii)	bis(1-oxopyridinium-2-sulfanylpropionate)	(001) interconnected layers	no	no	yes	NUHROY		P-1	3.30	
OJIKOH	cadmium(ii)	bis(D-camphor-10-sulfonate)	(001) stacked layers	no	no	no	LIJSOM		P2 ₁	8.10	
OKUZIF	magnesium(ii)	1H,1'H-5,5'-bitetrazole-1,1'-diolate	(001) interconnected layers	no	no	yes			Pbcn	2.52	

ONOSUG	cobalt(ii)	bis(4-carboxybenzenesulfonate)	(001) interconnected layers	[100] chain	dimer	no	ONOSUG	P-1	2.45	pillars connected through H-bonds
ONOTAN	zinc(ii)	bis(4-carboxybenzenesulfonate)	(001) interconnected layers	[100] chain	dimer	no	ONOSUG	P-1	2.85	pillars connected through H-bonds
ONOTER	iron(ii)	bis(4-carboxybenzenesulfonate)	(001) interconnected layers	[100] chain	dimer	no	ONOSUG	P-1	2.44	pillars connected through H-bonds
ORAQOP	magnesium(ii)	bis((4-chloro-2-methylphenoxy)acetate)	(100) stacked layers	[001] chain	no	no		C2/c	4.32	
PAHXIF	nickel(ii)	2,5-dicarboxylato-benzene-1,4-dicarboxylic acid	(010) interconnected layers	no	no	no		P2/m	4.40	anion with intramolecular H-bond
PAHXIF01	nickel(ii)	2,5-dicarboxylato-benzene-1,4-dicarboxylic acid	(100) interconnected layers	[001] zigzag chain	no	no	CAGVOV03	C2/c	3.17	anion with intramolecular H-bond
PIGRED	cobalt(ii)	bis(1-oxopyridinium-2-sulfanylpropionate)	(001) interconnected layers	no	no	yes	NUHROY	P-1	2.22	
POGGAW	manganese(ii)	bis(4-(2-hydroxybenzylideneamino)benzenesulfonate)	(010) interdigitated layers	no	no	no	POGGAW	P2 ₁ /c	2.65	anion with intramolecular H-bond
POTLOC	magnesium(ii)	3,6-bis(nitramido)-1,2,4,5-tetrazine	(001) interconnected layers	no	no	yes		P-1	4.06	
PUQWII	cobalt(ii)	bis(D-camphor-10-sulfonate)	(001) stacked layers	no	no	no	LIJSOM	P2 ₁	3.00	
PUQWOO	iron(ii)	bis(D-camphor-10-sulfonate)	(001) stacked layers	no	no	no	LIJSOM	P2 ₁	2.71	
PUQWUU	manganese(ii)	bis(D-camphor-10-sulfonate)	(001) stacked layers	no	no	no	LIJSOM	P2 ₁	6.85	
QEDCOR	iron(ii)	bis(trifluoromethanesulfonate)	(100) stacked layers	no	no	no	FAWBEM	C2/m	3.26	
QELXEK	nickel(ii)	bis(trifluoromethanesulfonate)	(001) stacked layers	no	no	no	BENBIG01	P-3m1	3.39	
QUKQES	manganese(ii)	bis(4-methylbenzenesulfonate)	(001) interdigitated layers	no	no	no	LIYYAT	P2 ₁ /n	3.80	
QUKQUI01	nickel(ii)	bis(4-methylbenzenesulfonate)	(001) interdigitated layers	no	no	no	LIYYAT	P2 ₁ /n	3.50	
RACBII	magnesium(ii)	bis(pyrazole-4-sulfonate)	(010) interconnected layers	no	[100] chain	yes		P-1	3.79	
RAKYOR	magnesium(ii)	naphthalene-1,5-disulfonate	(100) interconnected layers	(100) layer	no	no	FOGWUU	P2 ₁ /c	2.42	
RENREI	zinc(ii)	bis(1-oxopyridinium-2-sulfanylacetate)	(001) interconnected layers	no	no	yes	RENREI	P2 ₁ /c	4.91	
RENRII	cobalt(ii)	bis(1-oxopyridinium-2-sulfanylacetate)	(001) interconnected layers	no	no	yes	RENREI	P2 ₁ /c	6.39	
RENROS	nickel(ii)	bis(1-oxopyridinium-2-sulfanylacetate)	(001) interconnected layers	no	no	yes	RENREI	P2 ₁ /c	3.06	
RIHFEV	magnesium(ii)	bis(4-((4-(2-cyanoethyl)amino)phenyl)diazanyl)benzenesulfonate)	(100) interdigitated layers	no	[001] chain	no		C2/c	3.60	
ROXBEO	magnesium(ii)	bis((E)-4-((4-(dimethylamino)phenyl)diazanyl)benzenesulfonate)	(001) interdigitated layers	no	no	no	FAFYIX	P2 ₁ /c	2.55	
SESSUF	nickel(ii)	bis(4-nitrophenylsulfanylacetate)	(001) interconnected layers	no	no	yes		P-1	3.50	
SIYZII	copper(ii)	bis(4-chlorobenzenesulfonate)	(010) interdigitated layers	[100] chain	no	no		P2 ₁ /c	8.67	
SOFWIU	nickel(ii)	bis(4-(2-hydroxybenzylideneamino)benzenesulfonate)	(010) interdigitated layers	no	no	no	POGGAW	P2 ₁ /c	3.20	anion with intramolecular H-bond
SUVBOA	manganese(ii)	bis(4-styrenesulfonate)	(001) interdigitated layers	no	no	no	SUVBOA	P2 ₁ /c	7.70	
SUVBUG	cobalt(ii)	bis(4-styrenesulfonate)	(001) interdigitated layers	no	no	no	SUVBOA	P2 ₁ /c	5.01	
SUVCAN	nickel(ii)	bis(4-styrenesulfonate)	(001) interdigitated layers	no	no	no	SUVBOA	P2 ₁ /c	3.26	
TERKIK	cobalt(ii)	bis(2-aminotoluene-4-sulfonate)	(001) interconnected layers	no	no	yes		P2 ₁ /n	3.10	
TEVQIV	cobalt(ii)	bis(4-nitrophenylsulfanylacetate)	(001) interconnected layers	no	no	yes		P-1	3.95	
TITNIU	zinc(ii)	bis(4-(2-hydroxybenzylideneamino)benzenesulfonate)	(010) interdigitated layers	no	no	no	POGGAW	P2 ₁ /n	4.17	anion with intramolecular H-bond
TOKBUR	nickel(ii)	bis(2-carboxybenzenesulfonate)	(100) stacked layers	no	[001] zigzag chain	yes	TOKBUR	P2 ₁ /c	2.45	
TOKCAY	zinc(ii)	bis(2-carboxybenzenesulfonate)	(100) stacked layers	no	[001] zigzag chain	yes	TOKBUR	P2 ₁ /c	3.50	
TOLSCV	copper(ii)	bis(4-methylbenzenesulfonate)	(010) interdigitated layers	[100] chain	no	no		P2 ₁ /c	3.29	
TUFGIL	zinc(ii)	butane-1,4-diylbis(ammonio)bis(methylene))tetrakis(hydrogenphosphonate)	(001) interconnected layers	[100] chain	(001) layer	no		P-1	4.26	
TUJROG	nickel(ii)	3,3'-dicarboxybiphenyl-4,4'-dicarboxylate	(001) interconnected layers	no	no	no	DURPIQ	P-1	4.10	anion with intramolecular H-bond
UGURET	zinc(ii)	2,5-dicarboxylato-benzene-1,4-dicarboxylic acid	(100) interconnected layers	[001] zigzag chain	no	no	CAGVOV03	C2/c	2.74	anion with intramolecular H-bond
VELQEI	nickel(ii)	bis(dimethyl phosphate)	(100) stacked layers	(100) layer	no	no		P2 ₁ /c	2.41	
VENSAK	nickel(ii)	bis((E)-4-[[4-(dimethylamino)phenyl]diazanyl]benzenesulfonate)	(001) interdigitated layers	no	no	no	FAFYIX	P2 ₁ /c	3.19	
VEPSUE	vanadium(ii)	bis(trifluoromethanesulfonate)	(100) stacked layers	no	no	no	FAWBEM	C2/m	2.90	
VOPCEI	magnesium(ii)	bis(4-aminobenzenesulfonate)	(001) interconnected layers	no	no	yes		P2 ₁ /n	4.40	
VUYJII	magnesium(ii)	bis(2-((1-phenyl-1H-tetrazol-5-yl)sulfanyl)acetate)	(001) interdigitated layers	no	no	yes		P-1	3.20	
WABFOW	magnesium(ii)	bis(pyridinium-2,6-dicarboxylate)	(100) stacked layers	no	no	no		C2/m	5.40	
WABLIU10	cobalt(ii)	bis(benzenesulfonate)	(001) interdigitated layers	no	no	no	Isostructural	P2 ₁ /c	3.30	
WELQIQ	magnesium(ii)	2,2'-(1,3,6,8-tetraoxo-1,3,6,8-tetrahydrobenzo[Imn][3,8]phenanthroline-2,7-diyl)bis(ethane-1-sulfonate)	(001) interconnected layers	[1-10] chain	no	no	WELQIQ	P-1	3.39	
WELQOW	cobalt(ii)	2,2'-(1,3,6,8-tetraoxo-1,3,6,8-tetrahydrobenzo[Imn][3,8]phenanthroline-2,7-diyl)bis(ethane-1-sulfonate)	(001) interconnected layers	[1-10] chain	no	no	WELQIQ	P-1	5.69	
WIFZEQ	manganese(ii)	2,5-dicarboxylato-benzene-1,4-dicarboxylic acid	(100) interconnected layers	[001] zigzag chain	no	no	CAGVOV03	C2/c	5.79	anion with intramolecular H-bond
WIHPAF	zinc(ii)	bis(D-camphor-10-sulfonate)	(100) stacked layers	no	no	no	LIJSOM	P2 ₁	4.67	
XECJIY	magnesium(ii)	pyrazine-2,5-dicarboxylate	(001) interconnected layers	no	no	yes		P2 ₁ /c	5.16	
XEXXOS	chromium(iii)	hydrogen bis(phenylphosphonate)	(100) interdigitated layers	no	dimer	no		P2 ₁ 2 ₁ 2	6.27	anion with intramolecular H-bond
XIYMEY	cobalt(ii)	bis(4-(2-hydroxybenzylideneamino)benzenesulfonate)	(010) interdigitated layers	no	no	no	POGGAW	P2 ₁ /n	5.14	anion with intramolecular H-bond
YASHIK01	zinc(ii)	bis(6-hydroxynicotinate)	(001) interconnected layers	no	no	yes		C2/c	2.54	
YAXBEH	nickel(ii)	bis(1,7-dicarba-closo-dodecaborane(11)-1-phosphinate)	(001) stacked layers	no	no	no		C2/m	4.53	
YIDVIR	magnesium(ii)	bis(4-(2-hydroxybenzylideneamino)benzenesulfonate)	(010) interdigitated layers	no	no	no	POGGAW	P2 ₁ /n	2.39	anion with intramolecular H-bond
YOSYUB	cadmium(ii)	bis(4-methyl-5,7-dioxo-4,5,6,7-tetrahydro(1,2,3)triazolo(4,5-d)pyrimidin-3-ide)	(010) interconnected layers	no	dimer	yes		P-1	2.61	
YOSZAI	cadmium(ii)	bis(4,6-dimethyl-5,7-dioxo-4,5,6,7-tetrahydro(1,2,3)triazolo(4,5-d)pyrimidin-3-ide)	(001) interconnected layers	no	no	yes	YOSZAI	P-1	3.67	
YOSZEM	manganese(ii)	bis(4,6-dimethyl-5,7-dioxo-4,5,6,7-tetrahydro(1,2,3)triazolo(4,5-d)pyrimidin-3-ide)	(001) interconnected layers	no	no	yes	YOSZAI	P-1	3.45	
YOZTUE	magnesium(ii)	bis(5-(pyrazin-2-yl)tetrazol-1-ide)	(010) interconnected layers	no	no	yes		P-1	2.76	
ZEBSII	cobalt(ii)	piperazine-1,4-diyl-bis(methylenephosphinate)	(001) interconnected layers	no	no	yes		P-1	3.72	
ZNAQBS02	zinc(ii)	bis(benzenesulfonate)	(001) interdigitated layers	no	no	no	Isostructural	P2 ₁ /n	4.22	
ZZNLI01	magnesium(ii)	bis(4-methylbenzenesulfonate)	(001) interdigitated layers	no	no	no	LIYYAT	P2 ₁ /n	2.64	