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Crystallisation, thermal analysis and acetal protection activity of new layered Zn(II) hybrid polymorphs

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Figure S1. Selected bond distances (Å) and angles (°) in polymorph **1**

Octahedron around Zn		Tetrahedron around S1 and S2		Within the organic moieties	
Zn1-OW1	2.0823(3)	S1-O1	1.4957(3)	N1A-C2A	1.3521(2)
Zn1-OW1^{i}	2.0823(3)	S1-O2	1.4929(2)	N1A-C6A	1.3703(2)
Zn1-OW2	2.0874(5)	S1-O3	1.4656(5)	N2A-C2A	1.3353(2)
Zn1-OW2^{i}	2.0874(5)	S1-O4	1.4666(3)	C2A-C3A	1.4099(2)
Zn1-OW3	2.1119(3)	O2-S1-O1	107.223(8)	C3A-C4A	1.3695(2)
Zn1-OW3^{i}	2.1119(3)	O4-S1-O1	109.057(7)	C4A-C5A	1.4078(2)
Zn2-OW4	2.0742(3)	O3-S1-O1	109.802(8)	C5A-C6A	1.3641(2)
Zn2-OW4^{ii}	2.0742(3)	O4-S1-O2	110.652(1)	C6A-C7A	1.4911(1)
Zn2-OW5	2.0765(3)	O3-S1-O2	109.517(9)	C2A-N1A-C6A	123.382(1)
Zn2-OW5^{ii}	2.0765(3)	O3-S1-O4	110.528(9)	N2A-C2A-N1A	118.838(1)
Zn2-OW6	2.0852(6)	S2-O5	1.4771(2)	N2A-C2A-C3A	123.004(1)
Zn2-OW6^{ii}	2.0852(6)	S2-O6	1.4838(2)	N1A-C2A-C3A	118.158(1)
OW1^{i}-Zn1-OW1	179.986(4)	S2-O7	1.4876(3)	C4A-C3A-C2A	119.20(1)
OW1^{i}-Zn1-OW2^{i}	90.401(5)	S2-O8	1.4662(8)	C3A-C4A-C5A	121.013(1)
OW1-Zn1-OW2	89.599(5)	O8-S2-O5	110.527(8)	C6A-C5A-C4A	118.923(1)
OW1-Zn1-OW2^{i}	90.401(5)	O8-S2-O6	109.820(9)	C5A-C6A-N1A	119.313(1)
OW2-Zn1-OW2^{i}	179.993(6)	O5-S2-O6	110.652(1)	C5A-C6A-C7A	124.486(1)
OW1^{i}-Zn1-OW3	89.574(5)	O8-S2-O7	109.327(9)	N1A-C6A-C7A	116.201(1)
OW1-Zn1-OW3	90.426(5)	O5-S2-O7	108.754(7)	N1B-C2B	1.3524(2)
OW2-Zn1-OW3	88.424(6)	O6-S2-O7	109.919(9)	N1B-C6B	1.3668(2)
OW2^{i}-Zn1-OW3	91.576(6)			N2B-C2B	1.3372(2)
OW1^{i}-Zn1-OW3^{i}	90.426(5)			C2B-C3B	1.4107(2)
OW1-Zn1-OW3^{i}	89.574(5)			C3B-C4B	1.3688(2)
OW2-Zn1-OW3^{i}	91.576(6)			C4B-C5B	1.4108(2)
OW2^{i}-Zn1-OW3^{i}	88.424(6)			C5B-C6B	1.3658(2)
OW3-Zn1-OW3^{i}	179.996(6)			C6B-C7B	1.4962(1)
OW4^{ii}-Zn2-OW4	179.984(6)			C2B-N1B-C6B	123.570(1)
OW4^{ii}-Zn2-OW5	87.917(5)			N2B-C2B-N1B	118.769(1)
OW4-Zn2-OW5	92.083(5)			N2B-C2B-C3B	122.993(1)
OW4^{ii}-Zn2-OW5^{ii}	92.083(5)			N1B-C2B-C3B	118.238(1)
OW4-Zn2-OW5^{ii}	87.917(5)			C4B-C3B-C2B	118.998(1)
OW5-Zn2-OW5^{ii}	179.987(6)			C3B-C4B-C5B	121.118(2)
OW4^{ii}-Zn2-OW6^{ii}	90.933(6)			C6B-C5B-C4B	118.859(2)
OW4-Zn2-OW6^{ii}	89.067(6)			C5B-C6B-N1B	119.209(1)
OW5-Zn2-OW6^{ii}	93.756(5)			C5B-C6B-C7B	124.459(1)
OW5^{ii}-Zn2-OW6^{ii}	86.244(5)			N1B-C6B-C7B	116.332(1)
OW4^{ii}-Zn2-OW6	89.067(6)				
OW4-Zn2-OW6	90.933(6)				
OW5-Zn2-OW6	86.244(5)				
OW5^{ii}-Zn2-OW6	93.756(5)				
OW6^{ii}-Zn2-OW6	179.991(6)				

symmetry code: i = 1-x, 1-y, 1-z, ii = -x, 1-y, -z

Figure S2. Selected bond distances (Å) and angles (°) in polymorph **2**

Octahedron around Zn		Tetrahedron around S1, S2 and S3		Within the organic moieties	
Zn1-OW1	2.0946(3)	S1-O11	1.4761(2)	N1A-C6A	1.3502(1)
Zn1-OW1^{i}	2.0946(3)	S1-O21	1.4879(2)	N1A-C2A	1.3683(1)
Zn1-OW2	2.1024(2)	S1-O31	1.4673(2)	C2A-C3A	1.3602(2)
Zn1-OW2^{i}	2.1024(2)	S1-O41	1.4730(1)	C2A-C7A	1.4857(1)
Zn1-OW3	2.0591(4)	O11-S1-O21	109.518(1)	C3A-C4A	1.4088(1)
Zn1-OW3^{i}	2.0591(4)	O41-S1-O21	108.158(1)	C4A-C5A	1.3646(1)
Zn2-OW4	2.0935(3)	O31-S1-O21	109.231(1)	C5A-C6A	1.4034(2)
Zn2-OW5	2.1110(3)	O41-S1-O11	109.176(1)	C6A-N2A	1.3416(1)
Zn2-OW6	2.0753(1)	O31-S1-O11	110.052(1)	C6A-N1A-C2A	123.597(2)
Zn2-OW7	2.0461(1)	O31-S1-O41	110.673(1)	C3A-C2A-N1A	118.739(2)
Zn2-OW8	2.1034(3)	S2-O12	1.4755(2)	C3A-C2A-C7A	124.588(2)
Zn2-OW9	2.1036(3)	S2-O22	1.4654(2)	N1A-C2A-C7A	116.673(2)
OW3-Zn1-OW1^{i}	91.066(7)	S2-O32	1.4939(1)	C2AC3A-C4A	119.296(2)
OW3-Zn1-OW1	88.934(7)	S2-O42	1.4856(2)	C5A-C4A-C3A	120.940(2)
OW3^{i}-Zn1-OW2	87.281(7)	O22-S2-O12	110.418(1)	C4A-C5A-C6A	119.043(2)
OW3-Zn1-OW2	92.719(7)	O22-S2-O42	110.389(1)	N2A-C6A-N1A	118.651(2)
OW1^{i}-Zn1-OW2	89.042(7)	O12-S2-O42	108.868(1)	N2AC6A-C5A	122.970(2)
OW1-Zn1-OW2	90.958(7)	O22-S2-O32	109.968(1)	N1A-C6A-C7A	118.378(2)
OW3-Zn1-OW2^{i}	87.281(7)	O12-S2-O32	108.757(1)	N1B-C2B	1.3579(1)
OW-Zn1-OW2^{i}	89.042(78)	O42-S2-O32	108.392(9)	N1B-C6B	1.3711(1)
OW7-Zn2-OW6	177.325(6)	S3-O31	1.4690(2)	C2B-N2B	1.3390(8)
OW7-Zn2-OW4	87.069(6)	S3-O32	1.4940(2)	C2B-C3B	1.3983(2)
OW6-Zn2-OW4	90.277(6)	S3-O33	1.4825(2)	C3B-C4B	1.3744(1)
OW7-Zn2-OW8	91.645(6)	S3-O34	1.4606(2)	C4B-C5B	1.4109(1)
OW6-Zn2-OW8	88.768(6)	O34-S3-O31	109.88(12)	C5B-C6B	1.3588(2)
OW4-Zn2-OW8	91.638(7)	O34-S3-O33	111.00(11)	C6B-C7B	1.4897(1)
OW7-Zn2-OW9	86.426(7)	O31-S3-O33	109.36(12)	C2B-N1B-C6B	123.228(2)
OW6-Zn2-OW9	96.230(6)	O34-S3-O32	109.62(11)	N2B-C2B-N1B	117.806(2)
OW4-Zn2-OW9	173.478(8)	O31-S3-O32	109.68(11)	N2B-C2B-C3B	123.939(2)
OW8-Zn2-OW9	88.07(8)	O33-S3-O32	107.26(11)	N1B-C2B-C3B	118.253(2)
OW7-Zn2-OW5	91.429(6)			C4B-C3B-C2B	119.567(2)
OW6-Zn2-OW5	88.315(6)			C3B-C4B-C5B	120.407(2)
OW4-Zn2-OW5	91.828(7)			C6B-C5B-C4B	119.342(2)
OW8-Zn2-OW5	175.480(7)			C5B-C6B-N1B	119.200(2)
OW9-Zn2-OW5	88.815(7)			C5B-C6B-C7B	124.606(2)
				N1B-C6B-C7B	116.191(2)
				N1C-C2C	1.3434(1)
				N1C-C6C	1.3766(1)
				C2C-N2C	1.3388(8)
				C2C-C3C	1.4034(2)
				C3C-C4C	1.3704(1)
				C4C-C5C	1.4101(1)
				C5C-C6C	1.3541(2)
				C6C-C7C	1.4889(1)
				C2C-N1C-C6C	123.417(2)
				N2C-C2C-N1C	118.691(2)
				N2C-C2C-C3C	122.812(2)
				N1C-C2C-C3C	118.494(2)
				C4C-C3C-C2C	119.178(2)
				C3C-C4C-C5C	120.575(2)
				C6C-C5C-C4C	119.423(2)
				C5C-C6C-N1C	118.912(2)
				C5C-C6C-C7C	125.091(2)
				N1C-C6C-C7C	115.990(2)

Symmetry code: i = 1-x, 1-y, 1-z

Figure S3. Hydrogen bonding geometry (Å, °) for polymorph **1**

D–H···A	d(H···D) (Å)	d(H···A) (Å)	d(D···A) (Å)	∠ D–H···A(°)
N1A-H1A···O8	0.88	1.833	2.708	172.93
N2A-H2A···O6	0.87	2.069	2.947	176.19
N2A-H2B···O7^{i}	0.88	2.280	3.156	173.28
N1B-H1B···O3	0.88	1.850	2.724	172.05
N2B-H2C···O2	0.88	2.088	2.962	172.27
N2B-H2D···O4^{ii}	0.88	2.029	2.907	175.35
OW1-H1W1···O6	0.86	1.899	2.757	175.63
OW1-H2W1···O2	0.86	1.931	2.780	168.70
OW2-H1W2···O1	0.86	1.881	2.740	176.29
OW2-H2W2···O7^{iii}	0.86	1.879	2.732	171.60
OW3-H2W3···O1^{ii}	0.85	2.039	2.855	158.06
OW4-H1W4···O2	0.86	1.874	2.721	167.73
OW5-H1W5···O5^{i}	0.86	1.884	2.715	162.01
OW6-H1W6···O6	0.86	2.143	3.002	178.72
OW6-H1W6···O5	0.86	2.520	3.039	119.72
OW7-H1W7···O7^{iv}	0.86	1.852	2.703	170.23
OW7-H2W7···O1^{iii}	0.86	1.907	2.752	167.48
OW8-H1W8···O4^{ii}	0.86	1.889	2.725	163.61
OW8-H2W8···O5	0.86	1.966	2.822	173.50
OW3-H1W3···OW7	0.86	1.869	2.726	173.86
OW4-H2W4···OW8	0.86	1.857	2.714	174.24
OW5-H2W5···OW7^{iii}	0.86	1.983	2.798	157.76
OW6-H2W6···OW8^{v}	0.86	1.944	2.793	169.16
C3A-H3A···O8^{i}	0.95	2.50	3.356	150.6
C7A-H7C···O3^{vi}	0.98	2.60	3.232	122.5
C3B-H3B···O3^{ii}	0.95	2.63	3.473	148.5
C7B-H7E···O8^{vii}	0.98	2.65	3.374	130.5
C5A-H5A···OW2^{viii}	0.95	2.63	3.358	133.9
C5A-H5A···OW3^{viii}	0.95	2.56	3.453	157.4
C5B-H5B···OW4^{ix}	0.95	2.48	3.343	151.0

Symmetry code: i = x-1,y, z; ii = x+1, y, z; iii = -x+1, -y+1, -z+1; iv = -x+2, -y+1, -z+1; v = -x+1, -y+1, -z; vi = x+1, y+1, z; vii = x-1, y-1, z; viii = x, y+1, z; ix = -x, -y, -z.

Figure S4. Hydrogen bonding geometry (Å, °) for polymorph **2**

D–H···A	d(H···D) (Å)	d(H···A) (Å)	d(D···A) (Å)	∠ D–H···A(°)
N1A-H1A···O31	0.88	1.86	2.739	175.0
N2A-H2A1···O11	0.88	2.08	2.955	170.4
N2A-H2A2···O12^{i}	0.88	2.22	3.088	171.0
N1B-H1B···O22	0.88	1.85	2.729	172.7
N2B-H2B1···O24	0.88	2.127	2.997	169.6
N2B-H2B2···O21^{i}	0.88	2.01	2.878	171.2
N1C-H1C···O34	0.88	1.83	2.703	169.0
N2C-H2C1···O32	0.88	2.06	2.932	170.5
N2C-H2C2···O31^{ii}	0.88	2.00	2.878	177.4
O1W-H1W2···O11	0.86	2.52	3.348	161.1
O1W-H1W2···O14	0.86	2.27	2.928	133.2
O3W-H3W2···O32^{iii}	0.86	1.88	2.712	163.2
O4W-H4W1···O32	0.86	1.92	2.776	174.7
O4W-H4W2···O12	0.86	1.89	2.749	173.1
O5W-H5W2···O23^{iv}	0.86	1.89	2.838	162.1
O6W-H6W1···O32	0.86	1.90	2.748	167.7
O6W-H6W2···O11	0.86	1.87	2.731	178.0
O7W-H7W2···O24	0.86	1.89	2.741	168.4
O8W-H8W1···O33^{v}	0.86	2.09	2.870	151.4
O9W-H9W1···O33	0.86	1.98	2.805	161.0
O9W-H9W2···O24^{vi}	0.86	2.11	2.954	166.0
O11W-H1···O33	0.86	1.96	2.792	161.8
O9W-H9W2···O24^{vi}	0.86	2.11	2.954	166.0
O11W-H1···O33	0.86	1.96	2.792	161.8
O11W-H2···O12^{i}	0.86	1.86	2.711	173.2
O12W-H3···O23^{i}	0.86	1.99	2.797	156.7
O12W-H4···O21^{iv}	0.86	1.84	2.688	168.4
O13W-H5···O14^{iv}	0.86	1.94	2.795	169.9
O13W-H6···O31	0.86	1.87	2.700	160.9
O1W-H1W1···O13W^{iii}	0.86	1.95	2.790	166.6
O2W-H2W1···O11W^{iii}	0.86	2.00	2.809	155.6
O3W-H3W1···O13W^{vii}	0.86	1.87	2.721	171.9
O5W-H5W1···O11W	0.86	1.90	2.753	174.0
O7W-H7W1···O12W^{viii}	0.86	1.89	2.721	161.4
O8W-H8W2···O12W^{ii}	0.86	1.86	2.718	172.6
C3A-H3A···O3W^{viii}	0.95	2.53	3.387	149.9
C5A -H5A···O32^{iv}	0.95	2.55	3.410	151.1

Symmetry code: i = x+1, y, z; ii = x-1, y, z; iii = -x+1, -y+1, -z+1; iv = x+1, y, z; v = x-1, y, z; vi = -x, -y+1, -z+2; vii = -x+2, -y+1, -z+1; viii = -x+1, -y+1, -z+2; ix = -x+1, -y+2, -z+1.