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Supporting Information

Investigating the crystal structures of alkali and alkaline-earth metal salts of 2,5-(dianilino)terephthalic acid

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$[Mg(OH_2)_6(C_{20}H_{14}N_2O_4)]\cdot 2.8H_2O$ (**II**).

Table S3b. Atomic displacement parameters ($Å^2$) for $[Mg(OH_2)_6(C_{20}H_{14}N_2O_4)]\cdot 2.8H_2O$ (**II**).

Table S3c. Geometric parameters (Å, º) for $[Mg(OH_2)_6(C_{20}H_{14}N_2O_4)]\cdot 2.8H_2O$ (**II**).

Table S3d. Hydrogen-bond geometry (Å, º) for $[Mg(OH_2)_6(C_{20}H_{14}N_2O_4)]\cdot 2.8H_2O$ (**II**).

Figure S3b. Representation of hydrogen bonds (dashed lines) for $[Mg(OH_2)_6(C_{20}H_{14}N_2O_4)]\cdot 2.8H_2O$ (**II**) focused on both the Mg^{2+} (a) and the 2,5-(dianilino)terephthalate dianion (b) environments.

4. DFT calculations

Table S4a. Experimental, DFT optimized fractional atomic coordinates, and atomic displacement (in Å) during DFT optimization for $[(Li(OH_2)_3)_2(C_{20}H_{14}N_2O_4)]\cdot 2H_2O$ (**Ia**, form α).

Table S4b. Experimental, DFT optimized fractional atomic coordinates, and atomic displacement (in Å) during DFT optimization for $[(Li(OH_2)_4)_2(C_{20}H_{14}N_2O_4)]$ (**Ib**, form β).

Figure S4a. Total Density of states (DOS) for compound **Ia** (form α) (top) and compound **Ib** (form β) (bottom).

Figure S4b. Isosurface of the partial charge density calculated for the HOMO (left) and LUMO (right) for compound **Ia** (form α).

Figure S4c. Imaginary part of the calculated dielectric constant for compound **Ia** (form α) (top) and compound **Ib** (form β) (bottom).

References

1. S. P. Westrip, J. Appl. Crystallogr., 2010, 43, 920–925.
2. K. Brandenburg and H. Putz, DIAMOND version 3, 2005, Crystal Impact GbR, Bonn, Germany.

1. Compound $[(Li(OH_2)_3)_2(C_{20}H_{14}N_2O_4)]\cdot 2H_2O$ (**Ia**, form α)

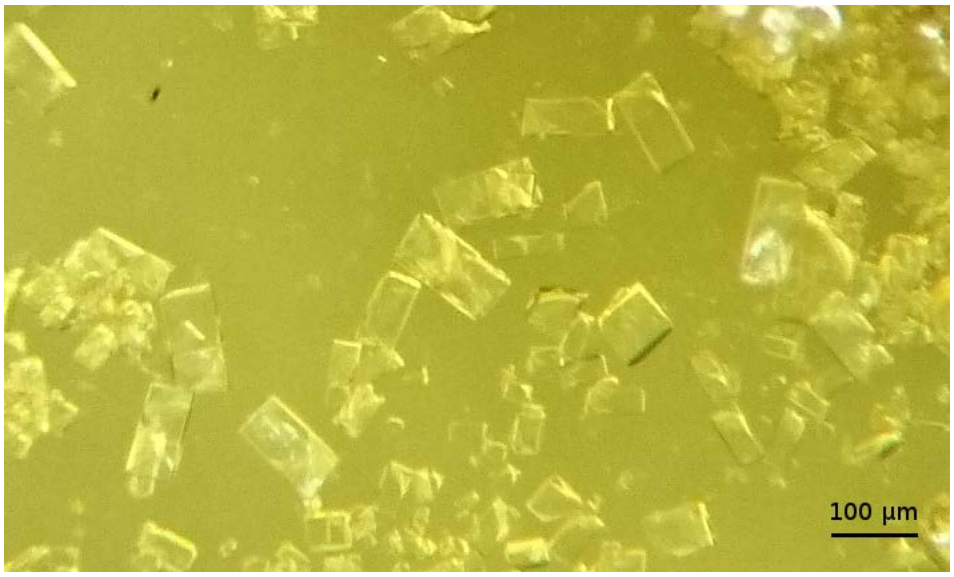

Figure S1a. Crystals of $[(Li(OH_2)_3)_2(C_{20}H_{14}N_2O_4)]\cdot 2H_2O$ (**Ia**, form α) in light yellow solution.

Table S1a. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for $[(Li(OH_2)_3)_2(C_{20}H_{14}N_2O_4)]\cdot 2H_2O$ (**Ia**, form α).

	x	*y*	*z*	U_{iso}*/U_{eq}
O11a	0.37413 (18)	0.75585 (17)	0.23134 (13)	0.0237 (6)
O12a	0.58286 (18)	0.58030 (17)	0.19178 (13)	0.0221 (5)
N21a	0.7710 (2)	0.2653 (2)	0.56877 (17)	0.0201 (6)
C1a	0.4833 (3)	0.5700 (2)	0.38413 (19)	0.0175 (7)
C2a	0.6312 (3)	0.3790 (2)	0.5343 (2)	0.0180 (7)
C3a	0.6100 (3)	0.4505 (2)	0.4207 (2)	0.0190 (7)
C11a	0.4786 (3)	0.6406 (2)	0.2611 (2)	0.0183 (7)
C21a	0.8441 (3)	0.1879 (3)	0.4645 (2)	0.0194 (7)
C22a	0.7453 (3)	0.0571 (3)	0.3722 (2)	0.0273 (8)
C23a	0.8177 (3)	-0.0141 (3)	0.2733 (2)	0.0353 (10)
C24a	0.9875 (3)	0.0447 (3)	0.2656 (2)	0.0331 (10)
C25a	1.0854 (3)	0.1755 (3)	0.3564 (2)	0.0346 (10)
C26a	1.0131 (3)	0.2469 (3)	0.4568 (2)	0.0289 (9)
H21a	0.734 (3)	0.201 (3)	0.618 (3)	0.043 (8)*
H22a	0.628003	0.016271	0.376832	0.0328*
H23a	0.750022	-0.104357	0.209919	0.0423*
H24a	1.036885	-0.005387	0.19741	0.0397*
H25a	1.201797	0.217037	0.350789	0.0415*
H26a	1.081053	0.33683	0.520383	0.0347*
H3a	0.686019	0.415904	0.365122	0.0228*
O1b	0.4557 (2)	0.72309 (19)	-0.02994 (18)	0.0252 (6)
O2b	0.2831 (3)	1.0645 (2)	0.07668 (17)	0.0308 (7)
O3b	0.0202 (2)	0.7220 (2)	-0.01426 (18)	0.0264 (6)
Li1b	0.2784 (5)	0.8319 (4)	0.0588 (4)	0.0275 (14)
H11b	0.507 (4)	0.672 (4)	0.041 (3)	0.077 (11)*
H12b	0.430 (3)	0.644 (4)	-0.101 (3)	0.055 (9)*
H21b	0.387 (4)	1.125 (4)	0.071 (3)	0.071 (10)*
H22b	0.187 (4)	1.119 (4)	0.060 (3)	0.065 (10)*
H31b	-0.002 (3)	0.675 (3)	0.054 (3)	0.058 (9)*
H32b	0.016 (4)	0.638 (4)	-0.079 (3)	0.066 (10)*
O1c	0.9540 (3)	0.5667 (2)	0.18607 (17)	0.0277 (6)
H11c	1.037 (4)	0.609 (4)	0.257 (3)	0.069 (11)*
H12c	0.837 (4)	0.570 (4)	0.200 (3)	0.083 (11)*

Table S1b. Atomic displacement parameters (Å^2) for $[(Li(OH_2)_3)_2(C_{20}H_{14}N_2O_4)]\cdot 2H_2O$ (**Ia**, form α).

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O11a	0.0304 (8)	0.0222 (9)	0.0222 (9)	0.0086 (7)	0.0110 (6)	0.0090 (7)
O12a	0.0283 (8)	0.0231 (8)	0.0188 (8)	0.0051 (6)	0.0115 (6)	0.0063 (7)
N21a	0.0241 (10)	0.0210 (10)	0.0177 (10)	0.0072 (8)	0.0083 (8)	0.0064 (8)
C1a	0.0190 (10)	0.0184 (11)	0.0144 (11)	-0.0018 (9)	0.0040 (8)	0.0028 (9)
C2a	0.0208 (11)	0.0147 (11)	0.0168 (11)	-0.0002 (8)	0.0037 (8)	0.0014 (9)
C3a	0.0225 (11)	0.0182 (11)	0.0171 (11)	0.0007 (9)	0.0081 (8)	0.0014 (9)
C11a	0.0215 (11)	0.0162 (11)	0.0165 (11)	-0.0017 (9)	0.0055 (8)	0.0017 (9)
C21a	0.0225 (11)	0.0207 (12)	0.0170 (11)	0.0063 (9)	0.0068 (9)	0.0075 (9)
C22a	0.0328 (13)	0.0243 (13)	0.0270 (13)	-0.0037 (10)	0.0128 (10)	0.0037 (10)
C23a	0.0541 (16)	0.0249 (14)	0.0289 (14)	-0.0034 (11)	0.0195 (12)	-0.0025 (11)
C24a	0.0505 (15)	0.0315 (15)	0.0266 (14)	0.0160 (12)	0.0225 (11)	0.0100 (12)
C25a	0.0311 (13)	0.0444 (16)	0.0325 (14)	0.0025 (11)	0.0155 (11)	0.0075 (12)
C26a	0.0287 (12)	0.0321 (14)	0.0251 (13)	-0.0020 (10)	0.0092 (10)	0.0005 (11)
O1b	0.0339 (9)	0.0222 (9)	0.0219 (9)	0.0015 (7)	0.0113 (7)	0.0048 (8)
O2b	0.0312 (10)	0.0237 (9)	0.0428 (11)	0.0051 (8)	0.0156 (8)	0.0122 (8)
O3b	0.0324 (9)	0.0216 (9)	0.0262 (9)	0.0020 (7)	0.0095 (7)	0.0054 (8)
Li1b	0.033 (2)	0.022 (2)	0.030 (2)	0.0032 (16)	0.0115 (17)	0.0061 (17)
O1c	0.0276 (9)	0.0293 (10)	0.0248 (10)	-0.0002 (7)	0.0082 (8)	0.0000 (8)

Table S1c. Geometric parameters (Å, º) for $[(Li(OH_2)_3)_2(C_{20}H_{14}N_2O_4)]\cdot 2H_2O$ (**Ia**, form α).

O11a—C11a	1.256 (2)	C24a—C25a	1.372 (3)
O11a—Li1b	1.959 (4)	C24a—H24a	0.95
O12a—C11a	1.277 (3)	C25a—C26a	1.391 (4)
N21a—C2a	1.415 (3)	C25a—H25a	0.95
N21a—C21a	1.445 (3)	C26a—H26a	0.95
N21a—H21a	0.90 (3)	O1b—Li1b	1.988 (4)
C1a—C2a^{i}	1.412 (3)	O1b—H11b	0.91 (3)
C1a—C3a	1.393 (3)	O1b—H12b	0.90 (3)
C1a—C11a	1.501 (3)	O2b—Li1b	1.907 (4)
C2a—C3a	1.390 (3)	O2b—H21b	0.94 (3)
C3a—H3a	0.95	O2b—H22b	0.84 (3)
C21a—C22a	1.381 (3)	O3b—Li1b	1.993 (4)
C21a—C26a	1.372 (3)	O3b—H31b	0.93 (3)
C22a—C23a	1.378 (4)	O3b—H32b	0.90 (3)
C22a—H22a	0.95	O1c—H11c	0.84 (3)
C23a—C24a	1.378 (4)	H12c—O1c	0.92 (4)
C23a—H23a	0.95		

C11a—O11a—Li1b	129.02 (18)	C23a—C24a—C25a	120.0 (2)
C2a—N21a—C21a	117.35 (17)	C23a—C24a—H24a	120.01
C2a—N21a—H21a	107.5 (15)	C25a—C24a—H24a	120.01
C21a—N21a—H21a	117.7 (16)	C24a—C25a—C26a	119.6 (2)
C2a^{i}—C1a—C3a	118.5 (2)	C24a—C25a—H25a	120.18
C2a^{i}—C1a—C11a	123.41 (18)	C26a—C25a—H25a	120.18
C3a—C1a—C11a	118.06 (19)	C21a—C26a—C25a	120.29 (19)
N21a—C2a—C1a^{i}	121.90 (19)	C21a—C26a—H26a	119.86
N21a—C2a—C3a	120.1 (2)	C25a—C26a—H26a	119.86
C1a^{i}—C2a—C3a	117.96 (18)	Li1b—O1b—H11b	91 (2)
C1a—C3a—C2a	123.5 (2)	Li1b—O1b—H12b	128.5 (17)
C1a—C3a—H3a	118.24	H11b—O1b—H12b	105 (3)
C2a—C3a—H3a	118.24	Li1b—O2b—H21b	121.5 (19)
O11a—C11a—O12a	123.0 (2)	Li1b—O2b—H22b	125 (2)
O11a—C11a—C1a	119.0 (2)	H21b—O2b—H22b	110 (3)
O12a—C11a—C1a	117.99 (18)	Li1b—O3b—H31b	106.4 (14)
N21a—C21a—C22a	120.9 (2)	Li1b—O3b—H32b	110.8 (18)
N21a—C21a—C26a	119.26 (17)	H31b—O3b—H32b	105 (3)
C22a—C21a—C26a	119.9 (2)	O11a—Li1b—O1b	98.34 (17)
C21a—C22a—C23a	119.7 (2)	O11a—Li1b—O2b	112.52 (18)
C21a—C22a—H22a	120.14	O11a—Li1b—O3b	102.3 (2)
C23a—C22a—H22a	120.14	O1b—Li1b—O2b	116.0 (2)
C22a—C23a—C24a	120.5 (2)	O1b—Li1b—O3b	111.55 (17)
C22a—C23a—H23a	119.76	O2b—Li1b—O3b	114.20 (19)
C24a—C23a—H23a	119.76		

Symmetry code: (i) -x+1, -y+1, -z+1.

Table S1d. Hydrogen-bond geometry (Å, º) for $[(Li(OH_2)_3)_2(C_{20}H_{14}N_2O_4)]\cdot 2H_2O$ (**Ia**, form α).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21*a*—H21*a*···O11*a*^{i}	0.90 (3)	1.98 (3)	2.679 (3)	133 (2)
C3*a*—H3*a*···O12*a*	0.95	2.40	2.759 (3)	101.85
C3*a*—H3*a*···C21*a*	0.95	2.44	2.809 (3)	102.58
O1*b*—H11*b*···O12*a*	0.91 (3)	1.82 (4)	2.716 (2)	172 (3)
O1*b*—H11*b*···C11*a*	0.91 (3)	2.46 (4)	3.221 (3)	142 (3)
O1*b*—H12*b*···O12*a*^{ii}	0.90 (3)	1.94 (3)	2.783 (2)	155 (3)
O2*b*—H21*b*···O1*b*^{iii}	0.94 (3)	1.89 (3)	2.807 (3)	165 (3)
O2*b*—H22*b*···O3*b*^{iv}	0.84 (3)	2.03 (3)	2.865 (2)	171 (3)
O3*b*—H31*b*···O1*c*^{v}	0.93 (3)	1.88 (3)	2.804 (3)	176 (3)
O3*b*—H32*b*···O1*c*^{ii}	0.90 (3)	1.95 (3)	2.827 (2)	166 (3)
O1*c*—H11*c*···N21*a*^{vi}	0.84 (3)	2.09 (3)	2.926 (2)	174 (3)
O1*c*—H12*c*···O12*a*	0.92 (4)	1.87 (3)	2.782 (2)	168 (3)

Symmetry codes: (i) -x+1, -y+1, -z+1; (ii) -x+1, -y+1, -z; (iii) -x+1, -y+2, -z; (iv) -x, -y+2, -z; (v) x-1, y, z; (vi) -x+2, -y+1, -z+1.

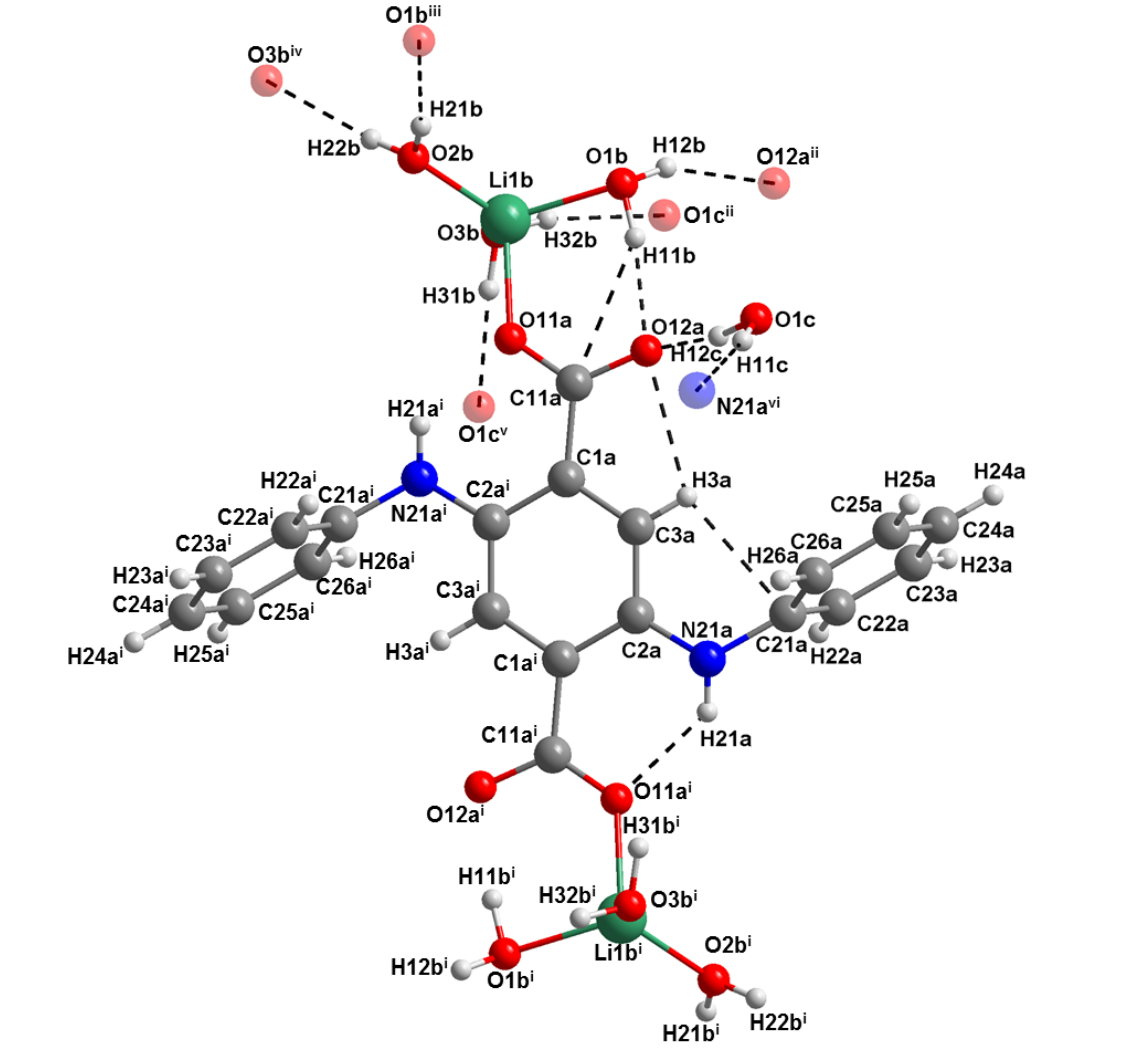

Figure S1b. Representation of hydrogen bonds (dashed lines) for $[(Li(OH_2)_3)_2(C_{20}H_{14}N_2O_4)]\cdot 2H_2O$ (**Ia**, form α).
Symmetry codes: (i) -x+1, -y+1, -z+1; (ii) -x+1, -y+1, -z; (iii) -x+1, -y+2, -z; (iv) -x, -y+2, -z; (v) x-1, y, z; (vi) -x+2, -y+1, -z+1.

2. Compound $[(Li(OH_2)_4)_2(C_{20}H_{14}N_2O_4)]$ (**Ib**, form β)

Figure S2a. Crystals of $[(Li(OH_2)_4)_2(C_{20}H_{14}N_2O_4)]$ (**Ib**, form β) in yellow solution.

Table S2a. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for $[(Li(OH_2)_4)_2(C_{20}H_{14}N_2O_4)]$ (**Ib**, form *β*).

	x	*y*	*z*	U_{iso}*/U_{eq}
O11a	0.20752 (13)	-0.4232 (3)	0.04897 (11)	0.0268 (6)
O12a	0.29928 (12)	-0.1274 (3)	0.01691 (9)	0.0214 (5)
N21a	0.00787 (17)	0.3872 (3)	-0.08811 (12)	0.0210 (7)
C1a	0.09908 (19)	-0.1144 (4)	0.01788 (13)	0.0182 (7)
C2a	0.00377 (19)	0.1948 (4)	-0.04507 (13)	0.0193 (8)
C3a	0.1005 (2)	0.0790 (4)	-0.02454 (13)	0.0198 (8)
C11a	0.20846 (19)	-0.2312 (4)	0.02927 (13)	0.0190 (8)
C21a	0.08091 (19)	0.4489 (4)	-0.14957 (14)	0.0202 (8)
C22a	0.0739 (2)	0.6586 (4)	-0.17849 (15)	0.0236 (8)
C23a	0.1410 (2)	0.7272 (5)	-0.24158 (15)	0.0300 (9)
C24a	0.2187 (2)	0.5929 (5)	-0.27634 (15)	0.0334 (9)
C25a	0.2246 (2)	0.3852 (5)	-0.24895 (16)	0.0346 (10)
C26a	0.1574 (2)	0.3130 (4)	-0.18668 (15)	0.0280 (9)
H3a	0.170585	0.134886	-0.040253	0.0238*
H21a	-0.056 (2)	0.477 (4)	-0.0826 (16)	0.039 (8)*
H22a	0.022501	0.754389	-0.154482	0.0284*
H23a	0.133754	0.868887	-0.261554	0.036*
H24a	0.26697	0.642761	-0.318111	0.0401*
H25a	0.27592	0.290219	-0.273471	0.0415*
H26a	0.163024	0.169256	-0.168777	0.0336*
O1b	0.48808 (16)	0.7008 (3)	0.09258 (11)	0.0252 (6)
O2b	0.37169 (15)	0.2848 (3)	0.05189 (11)	0.0256 (6)
O3b	0.61718 (16)	0.2613 (3)	0.13076 (12)	0.0272 (6)
O4b	0.45602 (17)	0.4400 (4)	0.25620 (12)	0.0312 (7)
Li1b	0.4753 (3)	0.4094 (7)	0.1362 (3)	0.0260 (14)
H11b	0.534 (2)	0.707 (5)	0.053 (2)	0.054 (10)*
H12b	0.420 (3)	0.758 (6)	0.067 (2)	0.070 (11)*
H21b	0.320 (3)	0.382 (6)	0.049 (2)	0.069 (12)*
H22b	0.341 (3)	0.149 (6)	0.042 (2)	0.067 (11)*
H31b	0.649 (3)	0.210 (6)	0.080 (2)	0.083 (12)*
H32b	0.669 (2)	0.318 (5)	0.1589 (19)	0.042 (10)*
H41b	0.421 (3)	0.541 (5)	0.286 (2)	0.074 (12)*
H42b	0.477 (3)	0.348 (6)	0.293 (2)	0.074 (13)*

Table S2b. Atomic displacement parameters (Å^2) for $[(Li(OH_2)_4)_2(C_{20}H_{14}N_2O_4)]$ (**Ib**, form *β*).

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O11a	0.0193 (10)	0.0201 (10)	0.0410 (10)	0.0039 (8)	0.0014 (8)	0.0006 (8)
O12a	0.0123 (9)	0.0246 (10)	0.0275 (9)	0.0008 (7)	0.0010 (7)	-0.0006 (7)
N21a	0.0174 (11)	0.0217 (12)	0.0243 (11)	0.0010 (10)	0.0039 (9)	0.0019 (10)
C1a	0.0172 (13)	0.0209 (14)	0.0164 (11)	0.0021 (11)	-0.0014 (10)	-0.0030 (10)
C2a	0.0182 (13)	0.0208 (14)	0.0189 (12)	0.0019 (11)	0.0018 (11)	-0.0002 (11)
C3a	0.0136 (13)	0.0258 (15)	0.0201 (12)	-0.0013 (11)	0.0016 (10)	-0.0028 (11)
C11a	0.0165 (13)	0.0230 (15)	0.0173 (12)	0.0021 (11)	-0.0020 (10)	-0.0018 (11)
C21a	0.0156 (12)	0.0229 (15)	0.0219 (12)	-0.0026 (11)	-0.0031 (11)	-0.0030 (11)
C22a	0.0210 (14)	0.0260 (16)	0.0236 (13)	0.0001 (12)	-0.0041 (11)	-0.0018 (11)
C23a	0.0274 (15)	0.0350 (17)	0.0271 (13)	-0.0072 (13)	-0.0084 (12)	0.0073 (13)
C24a	0.0235 (15)	0.056 (2)	0.0206 (13)	-0.0055 (14)	-0.0007 (12)	0.0091 (14)
C25a	0.0228 (15)	0.056 (2)	0.0252 (13)	0.0101 (14)	0.0055 (12)	0.0029 (14)
C26a	0.0264 (14)	0.0299 (16)	0.0276 (13)	0.0069 (13)	0.0006 (12)	0.0006 (12)
O1b	0.0216 (10)	0.0287 (11)	0.0252 (10)	0.0006 (9)	-0.0017 (9)	0.0014 (8)
O2b	0.0181 (10)	0.0207 (11)	0.0380 (11)	0.0021 (9)	-0.0012 (8)	-0.0024 (9)
O3b	0.0209 (10)	0.0350 (12)	0.0254 (10)	-0.0003 (9)	-0.0017 (9)	-0.0044 (9)
O4b	0.0371 (12)	0.0311 (12)	0.0255 (10)	0.0053 (10)	0.0027 (9)	0.0010 (10)
Li1b	0.023 (2)	0.024 (3)	0.031 (2)	0.0005 (19)	0.0019 (19)	-0.0010 (19)

Table S2c. Geometric parameters (Å, º) for $[(Li(OH_2)_4)_2(C_{20}H_{14}N_2O_4)]$ (**Ib**, form *β*).

O11a—C11a	1.248 (3)	C24a—C25a	1.379 (4)
O12a—C11a	1.288 (3)	C24a—H24a	0.95
N21a—C2a	1.394 (3)	C25a—C26a	1.377 (4)
N21a—C21a	1.391 (3)	C25a—H25a	0.95
C1a—C2a^{i}	1.411 (3)	C26a—H26a	0.95
C1a—C3a	1.394 (3)	O1b—Li1b	1.969 (5)
C1a—C11a	1.506 (3)	O1b—H11b	0.85 (3)
C2a—C3a	1.397 (3)	O2b—Li1b	1.969 (4)
C3a—H3a	0.95	O2b—H21b	0.87 (4)
C21a—C22a	1.400 (3)	O2b—H22b	0.94 (4)
C21a—C26a	1.397 (3)	O3b—Li1b	1.940 (5)
C22a—C23a	1.379 (3)	O3b—H32b	0.84 (3)
C22a—H22a	0.95	O4b—Li1b	1.953 (4)
C23a—C24a	1.385 (4)	O4b—H41b	0.91 (3)
C23a—H23a	0.95	O4b—H42b	0.86 (4)

C2a—N21a—C21a	128.6 (2)	C23a—C24a—H24a	120.74
C2a^{i}—C1a—C3a	119.1 (2)	C25a—C24a—H24a	120.74
C2a^{i}—C1a—C11a	123.3 (2)	C24a—C25a—C26a	121.2 (3)
C3a—C1a—C11a	117.5 (2)	C24a—C25a—H25a	119.4
N21a—C2a—C1a^{i}	120.5 (2)	C26a—C25a—H25a	119.4
N21a—C2a—C3a	121.8 (2)	C21a—C26a—C25a	120.7 (3)
C1a^{i}—C2a—C3a	117.6 (2)	C21a—C26a—H26a	119.66
C1a—C3a—C2a	123.2 (2)	C25a—C26a—H26a	119.66
C1a—C3a—H3a	118.39	Li1b—O1b—H11b	112 (2)
C2a—C3a—H3a	118.39	Li1b—O2b—H21b	101 (2)
O11a—C11a—O12a	122.9 (2)	Li1b—O2b—H22b	135 (2)
O11a—C11a—C1a	119.2 (2)	H21b—O2b—H22b	111 (3)
O12a—C11a—C1a	117.8 (2)	Li1b—O3b—H32b	114 (2)
N21a—C21a—C22a	117.7 (2)	Li1b—O4b—H41b	131 (2)
N21a—C21a—C26a	124.3 (2)	Li1b—O4b—H42b	125 (2)
C22a—C21a—C26a	118.0 (2)	H41b—O4b—H42b	104 (3)
C21a—C22a—C23a	120.5 (2)	O1b—Li1b—O2b	100.4 (2)
C21a—C22a—H22a	119.76	O1b—Li1b—O3b	110.7 (2)
C23a—C22a—H22a	119.76	O1b—Li1b—O4b	105.7 (2)
C22a—C23a—C24a	121.1 (3)	O2b—Li1b—O3b	108.1 (2)
C22a—C23a—H23a	119.44	O2b—Li1b—O4b	128.7 (2)
C24a—C23a—H23a	119.45	O3b—Li1b—O4b	102.8 (2)
C23a—C24a—C25a	118.5 (2)		

Symmetry code: (i) -x, -y, -z.

Table S2d. Hydrogen-bond geometry (Å, º) for $[(Li(OH_2)_4)_2(C_{20}H_{14}N_2O_4)]$ (**Ib**, form *β*).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3*a*—H3*a*···O12*a*	0.95	2.42	2.771 (3)	101.77
N21*a*—H21*a*···O11*a*^{i}	0.95 (3)	1.94 (3)	2.678 (3)	133 (2)
O1*b*—H11*b*···O2*b*^{ii}	0.85 (3)	2.06 (3)	2.901 (3)	173 (3)
O1*b*—H12*b*···O12*a*^{iii}	0.97 (3)	1.78 (3)	2.751 (2)	177 (3)
O2*b*—H21*b*···O11*a*^{iii}	0.87 (4)	1.82 (4)	2.687 (3)	176 (3)
O2*b*—H22*b*···O12*a*	0.94 (4)	1.85 (4)	2.784 (3)	172 (3)
O3*b*—H31*b*···O12*a*^{iv}	0.97 (4)	1.76 (4)	2.730 (3)	176 (3)
O3*b*—H31*b*···C11*a*^{iv}	0.97 (4)	2.48 (4)	3.359 (3)	151 (3)
O3*b*—H32*b*···C24*a*^{ii}	0.84 (3)	2.35 (3)	3.140 (3)	159 (3)
O4*b*—H41*b*···O3*b*^{v}	0.91 (3)	1.98 (3)	2.869 (3)	164 (3)
O4*b*—H42*b*···O1*b*^{vi}	0.86 (4)	2.09 (4)	2.913 (3)	162 (3)

Symmetry codes: (i) -x, -y, -z; (ii) -x+1, -y+1, -z; (iii) x, y+1, z; (iv) -x+1, -y, -z; (v) -x+1, y+1/2, -z+1/2; (vi) -x+1, y-1/2, -z+1/2.

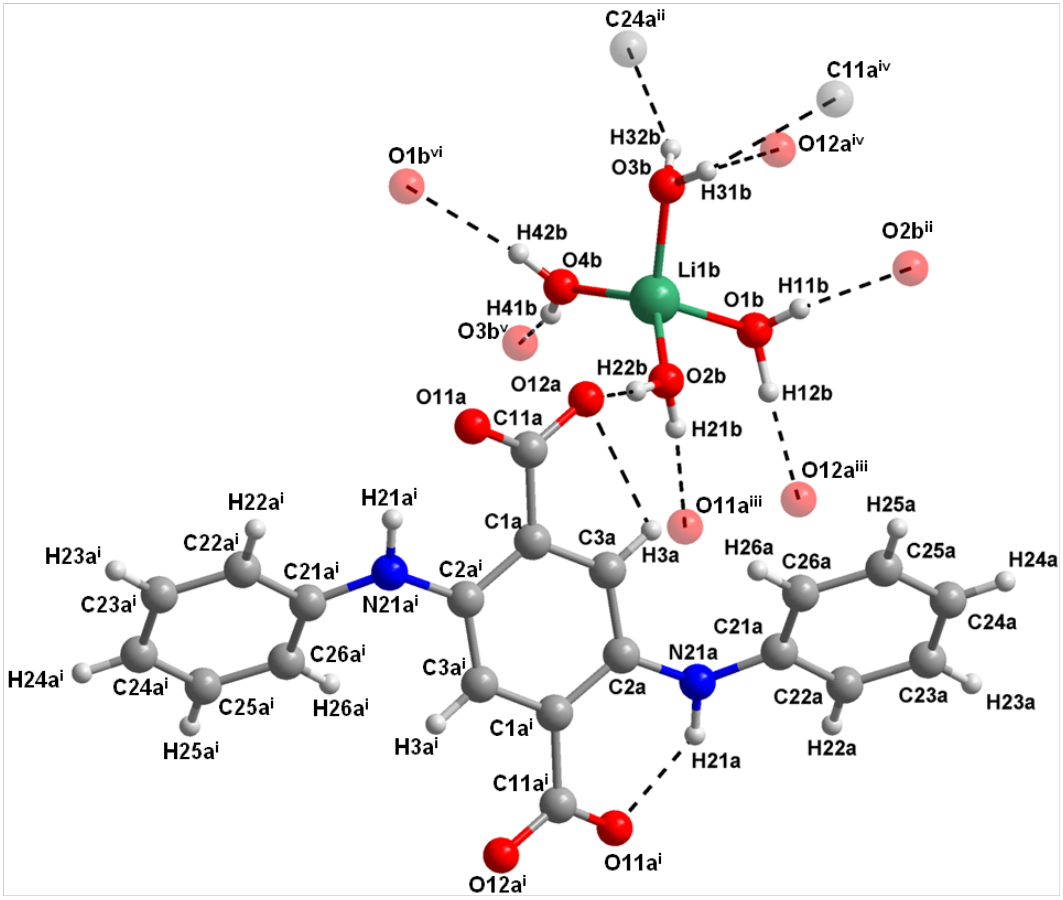

Figure S2b. Representation of hydrogen bonds (dashed lines) for $[(Li(OH_2)_4)_2(C_{20}H_{14}N_2O_4)]$ (**Ib**, form *β*).
Symmetry codes: (i) -x, -y, -z; (ii) -x+1, -y+1, -z; (iii) x, y+1, z; (iv) -x+1, -y, -z; (v) -x+1, y+1/2, -z+1/2; (vi) -x+1, y-1/2, -z+1/2.

3. Compound $[Mg(OH_2)_6(C_{20}H_{14}N_2O_4)]\cdot 2.8H_2O$ (**II**)

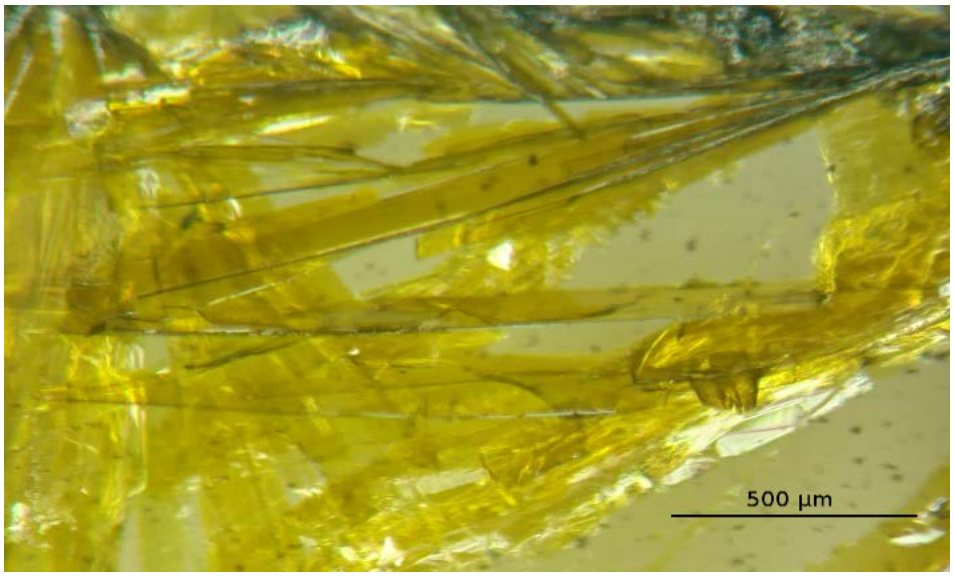

Figure S3a. Crystals of $[Mg(OH_2)_6(C_{20}H_{14}N_2O_4)]\cdot 2.8H_2O$ (**II**) in light yellow/green solution**.**

Table S3a. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for $[Mg(OH_2)_6(C_{20}H_{14}N_2O_4)]\cdot 2.8H_2O$ (**II**).

	x	*y*	*z*	U_{iso}*/U_{eq}
Mg1a	0.5	0	1	0.0183 (8)
O1a	0.5501 (2)	-0.06909 (18)	1.09770 (16)	0.0224 (13)
O2a	0.4548 (2)	-0.11186 (17)	0.90164 (16)	0.0256 (13)
O3a	0.3330 (2)	-0.05649 (19)	0.99118 (18)	0.0256 (13)
Mg1b	0.71038 (9)	0.20930 (8)	0.61074 (7)	0.0186 (5)
O1b	0.6517 (2)	0.2552 (2)	0.49300 (17)	0.0342 (14)
O2b	0.7321 (2)	0.33236 (17)	0.67989 (17)	0.0263 (13)
O3b	0.7646 (2)	0.16761 (18)	0.72782 (15)	0.0251 (13)
O4b	0.6836 (2)	0.08683 (17)	0.53895 (17)	0.0273 (13)
O5b	0.5373 (2)	0.15082 (19)	0.59115 (17)	0.0235 (13)
O6b	0.88038 (19)	0.26701 (19)	0.62818 (17)	0.0254 (13)
Mg1c	0.89496 (9)	0.39970 (8)	0.22477 (7)	0.0177 (5)
O1c	1.0066 (2)	0.51264 (18)	0.33133 (16)	0.0290 (13)
O2c	0.8278 (2)	0.47857 (19)	0.14907 (16)	0.0255 (13)
O3c	0.7933 (2)	0.28343 (17)	0.11772 (17)	0.0312 (13)
O4c	0.9598 (2)	0.31651 (18)	0.29722 (16)	0.0239 (13)
O5c	0.7664 (3)	0.3697 (2)	0.2644 (2)	0.0452 (18)
O6c	1.0192 (2)	0.4289 (2)	0.1772 (2)	0.0377 (16)
O11d	0.8206 (2)	0.60577 (17)	0.56807 (15)	0.0279 (12)
O12d	0.7684 (2)	0.46249 (18)	0.58551 (18)	0.0384 (14)
N21d	0.3481 (3)	0.3354 (2)	0.51513 (19)	0.0214 (15)
C1d	0.6187 (3)	0.5171 (2)	0.5296 (2)	0.0162 (16)
C2d	0.4226 (3)	0.4176 (2)	0.5081 (2)	0.0192 (16)
C3d	0.5403 (3)	0.4370 (2)	0.5353 (2)	0.0200 (17)
C11d	0.7446 (3)	0.5300 (3)	0.5636 (2)	0.0208 (17)
C21d	0.3767 (3)	0.2889 (2)	0.5834 (2)	0.0181 (16)
C22d	0.2991 (3)	0.1972 (2)	0.5684 (2)	0.0245 (18)
C23d	0.3187 (3)	0.1500 (3)	0.6351 (2)	0.031 (2)
C24d	0.4159 (3)	0.1912 (3)	0.7178 (2)	0.031 (2)
C25d	0.4935 (3)	0.2809 (3)	0.7330 (2)	0.0285 (19)
C26d	0.4740 (3)	0.3300 (3)	0.6668 (2)	0.0251 (18)
H3d	0.568348	0.393007	0.559074	0.024*
H21d	0.275 (3)	0.320 (3)	0.486 (2)	0.038 (12)*
H22d	0.232471	0.167258	0.511629	0.0294*
H23d	0.264533	0.088339	0.624026	0.0367*
H24d	0.429001	0.158259	0.763412	0.0375*
H25d	0.561139	0.309547	0.789341	0.0342*
H26d	0.527712	0.392043	0.678754	0.0301*
O11e	0.63548 (19)	0.39453 (16)	0.98505 (15)	0.0241 (12)
O12e	0.57542 (19)	0.25000 (16)	1.00013 (15)	0.0248 (12)
O41e	-0.00972 (19)	0.19139 (16)	0.82196 (15)	0.0235 (12)
O42e	0.04856 (19)	0.33693 (16)	0.80904 (14)	0.0209 (11)
N21e	0.4714 (3)	0.4550 (2)	0.88977 (19)	0.0203 (14)
N51e	0.1545 (3)	0.1348 (2)	0.92200 (19)	0.0209 (15)
C1e	0.4314 (3)	0.3092 (2)	0.9388 (2)	0.0169 (16)
C2e	0.3947 (3)	0.3737 (2)	0.8968 (2)	0.0157 (15)
C3e	0.2758 (3)	0.3556 (2)	0.8643 (2)	0.0168 (16)
C4e	0.1948 (3)	0.2792 (2)	0.8715 (2)	0.0152 (15)
C5e	0.2317 (3)	0.2142 (2)	0.9138 (2)	0.0169 (16)
C6e	0.3494 (3)	0.2314 (2)	0.9452 (2)	0.0167 (16)
C11e	0.5559 (3)	0.3194 (2)	0.9771 (2)	0.0172 (16)

C41e	0.0687 (3)	0.2672 (2)	0.8319 (2)	0.0164 (16)
C21e	0.4454 (3)	0.4995 (2)	0.8202 (2)	0.0164 (16)
C22e	0.5148 (3)	0.5932 (2)	0.8358 (2)	0.0217 (17)
C23e	0.4986 (3)	0.6372 (3)	0.7662 (2)	0.0253 (18)
C24e	0.4113 (3)	0.5901 (3)	0.6803 (2)	0.0267 (19)
C25e	0.3407 (3)	0.4979 (3)	0.6649 (2)	0.0258 (18)
C26e	0.3575 (3)	0.4526 (2)	0.7339 (2)	0.0218 (17)
C51e	0.1810 (3)	0.0906 (2)	0.9927 (2)	0.0172 (16)
C52e	0.2756 (3)	0.1356 (3)	1.0770 (2)	0.0250 (18)
C53e	0.2955 (3)	0.0912 (3)	1.1459 (2)	0.0280 (19)
C54e	0.2220 (3)	0.0008 (3)	1.1334 (2)	0.030 (2)
C55e	0.1275 (3)	-0.0451 (3)	1.0497 (2)	0.029 (2)
C56e	0.1076 (3)	-0.0009 (2)	0.9798 (2)	0.0246 (18)
H3e	0.249611	0.398375	0.835614	0.0201*
H6e	0.375229	0.187804	0.972356	0.02*
H21e	0.539 (3)	0.468 (2)	0.922 (2)	0.010 (9)*
H22e	0.573837	0.627053	0.894831	0.0261*
H23e	0.548032	0.700572	0.777621	0.0304*
H24e	0.400047	0.620495	0.632659	0.032*
H25e	0.279834	0.464946	0.606166	0.0309*
H26e	0.308318	0.389128	0.721971	0.0262*
H51e	0.084 (3)	0.120 (3)	0.891 (2)	0.034 (12)*
H52e	0.327321	0.197964	1.087419	0.03*
H53e	0.360987	0.12337	1.20284	0.0336*
H54e	0.235943	-0.02936	1.181212	0.0361*
H55e	0.075738	-0.107296	1.039985	0.0352*
H56e	0.043172	-0.033665	0.922557	0.0295*
O11f	0.42731 (19)	0.21867 (17)	0.38433 (15)	0.0269 (12)
O12f	0.37975 (19)	0.08077 (16)	0.41478 (15)	0.0240 (12)
O41f	-0.21893 (19)	-0.00043 (17)	0.21802 (15)	0.0261 (12)
O42f	-0.16571 (19)	0.13435 (16)	0.18247 (16)	0.0267 (12)
N21f	0.2569 (3)	0.2666 (2)	0.2776 (2)	0.0222 (15)
N51f	-0.0510 (3)	-0.0579 (2)	0.31103 (19)	0.0212 (14)
C1f	0.2245 (3)	0.1247 (2)	0.3337 (2)	0.0165 (16)
C2f	0.1830 (3)	0.1855 (2)	0.2862 (2)	0.0171 (16)
C3f	0.0630 (3)	0.1621 (2)	0.2500 (2)	0.0162 (15)
C4f	-0.0158 (3)	0.0845 (2)	0.2583 (2)	0.0152 (15)
C5f	0.0248 (3)	0.0230 (2)	0.3041 (2)	0.0165 (16)
C6f	0.1445 (3)	0.0452 (2)	0.3390 (2)	0.0186 (16)
C11f	0.3516 (3)	0.1431 (2)	0.3795 (2)	0.0189 (17)
C41f	-0.1420 (3)	0.0711 (2)	0.2170 (2)	0.0185 (16)
C21f	0.2251 (3)	0.3129 (2)	0.2097 (2)	0.0175 (16)
C22f	0.2845 (3)	0.4087 (2)	0.2289 (2)	0.0231 (17)
C23f	0.2607 (3)	0.4558 (3)	0.1610 (2)	0.0274 (19)
C24f	0.1761 (3)	0.4086 (3)	0.0748 (2)	0.0267 (19)
C25f	0.1155 (3)	0.3135 (3)	0.0553 (2)	0.0281 (19)
C26f	0.1402 (3)	0.2664 (2)	0.1218 (2)	0.0225 (17)
C51f	-0.0260 (3)	-0.1031 (2)	0.3801 (2)	0.0186 (17)
C52f	0.0633 (3)	-0.0584 (3)	0.4669 (2)	0.0316 (19)
C53f	0.0789 (3)	-0.1051 (3)	0.5341 (2)	0.034 (2)
C54f	0.0067 (3)	-0.1967 (3)	0.5174 (2)	0.030 (2)
C55f	-0.0816 (3)	-0.2417 (3)	0.4314 (2)	0.0299 (19)
C56f	-0.0978 (3)	-0.1960 (2)	0.3634 (2)	0.0229 (17)
H3f	0.033747	0.201778	0.217842	0.0195*
H6f	0.17286	0.003582	0.368159	0.0223*
H21f	0.327 (3)	0.287 (3)	0.313 (2)	0.035 (12)*

H22f	0.341561	0.44224	0.288579	0.0277*
H23f	0.303391	0.520824	0.17458	0.0329*
H24f	0.159312	0.440929	0.029019	0.0321*
H25f	0.056692	0.280552	-0.004091	0.0337*
H26f	0.098508	0.201078	0.107313	0.027*
H51f	-0.121 (3)	-0.073 (2)	0.275 (2)	0.029 (11)*
H52f	0.113955	0.004837	0.479879	0.0379*
H53f	0.140347	-0.073458	0.592907	0.041*
H54f	0.017409	-0.228265	0.56418	0.0354*
H55f	-0.131715	-0.305085	0.41884	0.0359*
H56f	-0.158767	-0.228317	0.304575	0.0275*
O1g	0.5203 (2)	0.0242 (2)	0.35683 (18)	0.0302 (14)
O1h	0.8169 (3)	0.3582 (2)	0.96763 (19)	0.0415 (17)
O1i	0.6616 (3)	0.10555 (19)	0.27474 (18)	0.0349 (15)
O1j	0.7836 (2)	0.2813 (2)	0.39862 (19)	0.0388 (15)
O1k	0.9853 (3)	0.58111 (19)	0.49029 (17)	0.0362 (14)
O1l	0.6826 (3)	0.1760 (3)	0.8535 (2)	0.052 (2)
O1m	0.9074 (2)	0.40157 (18)	0.85087 (17)	0.0272 (13)
H11a	0.519 (3)	-0.1265 (5)	1.076 (2)	0.052 (14)*
H12a	0.6225 (10)	-0.049 (2)	1.130 (2)	0.061 (15)*
H21a	0.439 (4)	-0.1634 (11)	0.915 (2)	0.081 (18)*
H22a	0.421 (3)	-0.116 (2)	0.8462 (5)	0.055 (14)*
H31a	0.315 (3)	-0.0237 (19)	1.0196 (17)	0.028 (11)*
H32a	0.282 (2)	-0.082 (3)	0.9376 (10)	0.09 (2)*
H11b	0.5833 (18)	0.237 (4)	0.452 (3)	0.132 (18)*
H12b	0.678 (5)	0.3131 (5)	0.509 (4)	0.132 (18)*
H21b	0.775 (3)	0.347 (2)	0.7357 (4)	0.049 (14)*
H22b	0.744 (4)	0.3772 (15)	0.656 (2)	0.086 (19)*
H31b	0.735 (2)	0.167 (3)	0.7634 (15)	0.047 (13)*
H32b	0.8352 (11)	0.176 (3)	0.7539 (17)	0.062 (16)*
H41b	0.644 (3)	0.072 (2)	0.4827 (3)	0.063 (16)*
H42b	0.673 (4)	0.0412 (15)	0.562 (2)	0.073 (17)*
H51b	0.511 (3)	0.180 (3)	0.615 (2)	0.066 (16)*
H52b	0.492 (3)	0.124 (3)	0.5367 (8)	0.075 (18)*
H61b	0.9302 (19)	0.298 (2)	0.6806 (9)	0.038 (12)*
H62b	0.907 (2)	0.240 (2)	0.6019 (18)	0.050 (14)*
H11c	1.0761 (13)	0.519 (3)	0.359 (2)	0.069 (17)*
H12c	0.983 (3)	0.533 (3)	0.3650 (19)	0.081 (18)*
H21c	0.7656 (18)	0.453 (2)	0.1008 (13)	0.051 (14)*
H22c	0.862 (3)	0.5358 (6)	0.156 (2)	0.075 (18)*
H31c	0.7236 (10)	0.273 (2)	0.084 (2)	0.048 (13)*
H32c	0.801 (3)	0.2363 (14)	0.134 (3)	0.072 (17)*
H41c	1.0302 (9)	0.3410 (19)	0.3360 (18)	0.047 (13)*
H42c	0.938 (3)	0.2608 (8)	0.273 (2)	0.051 (14)*
H51c	0.766 (3)	0.340 (2)	0.303 (2)	0.036 (12)*
H52c	0.720 (3)	0.395 (3)	0.254 (3)	0.080 (18)*
H61c	1.066 (3)	0.404 (2)	0.186 (3)	0.071 (17)*
H62c	1.042 (3)	0.4801 (16)	0.165 (3)	0.078 (18)*
H11g	0.484 (3)	0.050 (2)	0.372 (3)	0.061 (15)*
H12g	0.490 (3)	-0.0335 (4)	0.349 (3)	0.09 (2)*
H11h	0.765 (3)	0.374 (3)	0.968 (3)	0.080 (18)*
H12h	0.856 (4)	0.349 (4)	1.0169 (16)	0.10 (2)*
H11i	0.612 (3)	0.072 (3)	0.289 (3)	0.082 (19)*
H12i	0.693 (5)	0.077 (3)	0.256 (5)	0.19 (4)*
H11j	0.757 (5)	0.225 (4)	0.357 (3)	0.13 (3)*
H12j	0.740 (5)	0.268 (4)	0.424 (4)	0.20 (4)*

H11k	0.935 (4)	0.576 (5)	0.509 (4)	0.19 (4)*
H12k	1.052 (2)	0.620 (4)	0.527 (3)	0.2*
H11l	0.655 (4)	0.136 (2)	0.877 (3)	0.09 (2)*
H12l	0.727 (6)	0.2280 (19)	0.890 (3)	0.20 (4)*
H11m	0.947 (3)	0.374 (3)	0.843 (3)	0.070 (17)*
H12m	0.890 (4)	0.389 (3)	0.893 (2)	0.068 (17)*

Table S3b. Atomic displacement parameters (Å^2) for $[Mg(OH_2)_6(C_{20}H_{14}N_2O_4)]\cdot 2.8H_2O$ (**II**).

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1a	0.0141 (9)	0.0205 (10)	0.0202 (8)	0.0085 (8)	0.0059 (7)	0.0078 (7)
O1a	0.0176 (15)	0.0205 (16)	0.0236 (14)	0.0084 (12)	0.0034 (12)	0.0061 (12)
O2a	0.0285 (16)	0.0248 (16)	0.0215 (15)	0.0105 (13)	0.0099 (13)	0.0054 (12)
O3a	0.0221 (15)	0.0278 (16)	0.0286 (15)	0.0121 (13)	0.0113 (13)	0.0068 (13)
Mg1b	0.0146 (6)	0.0207 (7)	0.0201 (6)	0.0080 (5)	0.0060 (5)	0.0088 (5)
O1b	0.0179 (15)	0.056 (2)	0.0237 (14)	0.0115 (15)	0.0065 (12)	0.0189 (15)
O2b	0.0281 (16)	0.0250 (15)	0.0282 (16)	0.0155 (12)	0.0107 (14)	0.0096 (13)
O3b	0.0181 (15)	0.0342 (17)	0.0267 (13)	0.0130 (13)	0.0103 (12)	0.0148 (12)
O4b	0.0269 (15)	0.0286 (16)	0.0245 (15)	0.0120 (13)	0.0094 (13)	0.0065 (13)
O5b	0.0177 (14)	0.0281 (16)	0.0272 (15)	0.0110 (13)	0.0105 (13)	0.0087 (12)
O6b	0.0139 (14)	0.0337 (17)	0.0240 (14)	0.0084 (13)	0.0062 (13)	0.0031 (13)
Mg1c	0.0136 (6)	0.0184 (7)	0.0205 (6)	0.0078 (5)	0.0060 (5)	0.0048 (5)
O1c	0.0218 (16)	0.0293 (16)	0.0292 (14)	0.0132 (13)	0.0041 (13)	-0.0003 (12)
O2c	0.0205 (15)	0.0197 (16)	0.0261 (15)	0.0091 (13)	0.0005 (13)	0.0039 (12)
O3c	0.0238 (17)	0.0231 (16)	0.0315 (15)	0.0130 (12)	-0.0044 (13)	0.0035 (13)
O4c	0.0195 (16)	0.0213 (16)	0.0237 (14)	0.0095 (12)	0.0023 (12)	0.0030 (12)
O5c	0.044 (2)	0.062 (2)	0.067 (2)	0.0385 (18)	0.0425 (18)	0.0436 (19)
O6c	0.0410 (18)	0.0335 (19)	0.067 (2)	0.0241 (16)	0.0412 (17)	0.0256 (16)
O11d	0.0153 (14)	0.0250 (15)	0.0339 (14)	0.0061 (12)	0.0038 (12)	0.0097 (12)
O12d	0.0208 (15)	0.0390 (18)	0.0634 (19)	0.0188 (14)	0.0172 (14)	0.0348 (15)
N21d	0.0110 (17)	0.0211 (18)	0.0261 (17)	0.0052 (14)	0.0030 (14)	0.0104 (14)
C1d	0.0161 (19)	0.019 (2)	0.0134 (17)	0.0083 (16)	0.0059 (15)	0.0043 (15)
C2d	0.020 (2)	0.021 (2)	0.0138 (17)	0.0080 (17)	0.0055 (15)	0.0035 (15)
C3d	0.021 (2)	0.021 (2)	0.0192 (18)	0.0108 (17)	0.0080 (16)	0.0075 (15)
C11d	0.020 (2)	0.024 (2)	0.0203 (18)	0.0117 (18)	0.0078 (16)	0.0089 (16)
C21d	0.0175 (19)	0.020 (2)	0.0223 (18)	0.0113 (17)	0.0108 (16)	0.0094 (16)
C22d	0.025 (2)	0.020 (2)	0.024 (2)	0.0075 (18)	0.0100 (17)	0.0033 (17)
C23d	0.038 (3)	0.022 (2)	0.033 (2)	0.009 (2)	0.020 (2)	0.0137 (18)
C24d	0.042 (3)	0.030 (2)	0.032 (2)	0.019 (2)	0.021 (2)	0.0192 (19)
C25d	0.032 (2)	0.032 (2)	0.0204 (19)	0.014 (2)	0.0086 (18)	0.0106 (18)
C26d	0.021 (2)	0.024 (2)	0.028 (2)	0.0076 (18)	0.0093 (17)	0.0088 (17)
O11e	0.0139 (13)	0.0211 (14)	0.0296 (14)	0.0039 (12)	0.0051 (11)	0.0083 (11)
O12e	0.0150 (13)	0.0181 (14)	0.0357 (14)	0.0072 (11)	0.0054 (11)	0.0090 (12)
O41e	0.0145 (13)	0.0212 (15)	0.0317 (14)	0.0059 (12)	0.0076 (11)	0.0131 (11)
O42e	0.0163 (13)	0.0182 (14)	0.0273 (13)	0.0099 (11)	0.0060 (11)	0.0088 (11)
N21e	0.0091 (17)	0.0221 (18)	0.0238 (16)	0.0040 (14)	0.0032 (14)	0.0099 (14)
N51e	0.0137 (18)	0.0231 (19)	0.0239 (16)	0.0083 (15)	0.0050 (14)	0.0115 (14)
C1e	0.0161 (19)	0.018 (2)	0.0159 (17)	0.0076 (16)	0.0062 (15)	0.0046 (15)
C2e	0.0153 (19)	0.0152 (19)	0.0151 (17)	0.0055 (16)	0.0061 (15)	0.0035 (15)
C3e	0.0192 (19)	0.018 (2)	0.0148 (17)	0.0102 (16)	0.0068 (15)	0.0080 (15)
C4e	0.0149 (18)	0.0160 (19)	0.0139 (16)	0.0066 (16)	0.0053 (15)	0.0038 (14)
C5e	0.0154 (19)	0.018 (2)	0.0152 (17)	0.0047 (16)	0.0064 (15)	0.0035 (15)
C6e	0.0175 (19)	0.0141 (19)	0.0161 (17)	0.0077 (15)	0.0045 (15)	0.0025 (14)
C11e	0.0136 (19)	0.019 (2)	0.0159 (17)	0.0071 (16)	0.0028 (15)	0.0066 (15)
C41e	0.0150 (19)	0.020 (2)	0.0127 (17)	0.0068 (17)	0.0050 (15)	0.0038 (15)
C21e	0.0166 (19)	0.020 (2)	0.0165 (17)	0.0099 (16)	0.0089 (15)	0.0054 (15)
C22e	0.021 (2)	0.021 (2)	0.0229 (19)	0.0078 (17)	0.0100 (17)	0.0049 (16)
C23e	0.028 (2)	0.018 (2)	0.033 (2)	0.0082 (18)	0.0178 (19)	0.0084 (17)
C24e	0.032 (2)	0.030 (2)	0.030 (2)	0.0183 (19)	0.0193 (19)	0.0168 (18)
C25e	0.026 (2)	0.031 (2)	0.0187 (19)	0.0109 (19)	0.0097 (17)	0.0079 (17)
C26e	0.022 (2)	0.019 (2)	0.0250 (19)	0.0051 (17)	0.0131 (17)	0.0064 (16)
C51e	0.0195 (19)	0.018 (2)	0.0228 (18)	0.0125 (16)	0.0132 (16)	0.0090 (16)

C52e	0.025 (2)	0.020 (2)	0.0244 (19)	0.0035 (18)	0.0098 (17)	0.0053 (17)
C53e	0.034 (2)	0.030 (2)	0.021 (2)	0.017 (2)	0.0104 (18)	0.0099 (18)
C54e	0.041 (2)	0.029 (2)	0.031 (2)	0.020 (2)	0.020 (2)	0.0186 (19)
C55e	0.033 (2)	0.023 (2)	0.039 (2)	0.0107 (19)	0.021 (2)	0.0154 (19)
C56e	0.028 (2)	0.023 (2)	0.024 (2)	0.0092 (18)	0.0132 (18)	0.0072 (17)
O11f	0.0131 (13)	0.0293 (16)	0.0323 (14)	0.0064 (12)	0.0054 (11)	0.0132 (12)
O12f	0.0159 (13)	0.0235 (15)	0.0322 (14)	0.0106 (12)	0.0075 (11)	0.0120 (12)
O41f	0.0121 (13)	0.0293 (16)	0.0327 (14)	0.0072 (12)	0.0058 (11)	0.0159 (12)
O42f	0.0155 (14)	0.0200 (14)	0.0391 (15)	0.0092 (12)	0.0049 (12)	0.0106 (12)
N21f	0.0132 (18)	0.0228 (19)	0.0255 (17)	0.0038 (15)	0.0061 (15)	0.0118 (14)
N51f	0.0104 (17)	0.0211 (18)	0.0230 (16)	0.0038 (14)	0.0007 (14)	0.0092 (14)
C1f	0.0128 (18)	0.019 (2)	0.0175 (17)	0.0082 (16)	0.0054 (15)	0.0044 (15)
C2f	0.0175 (19)	0.019 (2)	0.0140 (17)	0.0070 (16)	0.0067 (15)	0.0032 (15)
C3f	0.0144 (19)	0.0168 (19)	0.0159 (17)	0.0077 (16)	0.0039 (15)	0.0058 (14)
C4f	0.0110 (18)	0.018 (2)	0.0133 (16)	0.0046 (15)	0.0039 (14)	0.0002 (14)
C5f	0.0153 (19)	0.017 (2)	0.0166 (17)	0.0077 (16)	0.0054 (15)	0.0068 (15)
C6f	0.0163 (19)	0.021 (2)	0.0179 (17)	0.0109 (16)	0.0043 (15)	0.0077 (15)
C11f	0.017 (2)	0.025 (2)	0.0162 (17)	0.0101 (18)	0.0073 (15)	0.0067 (16)
C41f	0.018 (2)	0.020 (2)	0.0163 (17)	0.0105 (17)	0.0043 (15)	0.0040 (15)
C21f	0.0161 (19)	0.019 (2)	0.0205 (18)	0.0058 (16)	0.0120 (16)	0.0071 (15)
C22f	0.022 (2)	0.023 (2)	0.0199 (19)	0.0082 (17)	0.0066 (16)	0.0039 (16)
C23f	0.030 (2)	0.020 (2)	0.032 (2)	0.0086 (19)	0.0150 (19)	0.0102 (18)
C24f	0.033 (2)	0.031 (2)	0.026 (2)	0.0184 (19)	0.0156 (18)	0.0172 (18)
C25f	0.029 (2)	0.034 (2)	0.0183 (19)	0.010 (2)	0.0098 (17)	0.0058 (18)
C26f	0.026 (2)	0.019 (2)	0.0234 (19)	0.0080 (18)	0.0127 (17)	0.0056 (16)
C51f	0.0174 (19)	0.022 (2)	0.0250 (19)	0.0123 (17)	0.0126 (16)	0.0120 (16)
C52f	0.026 (2)	0.023 (2)	0.028 (2)	-0.0021 (18)	0.0051 (18)	0.0074 (18)
C53f	0.029 (2)	0.035 (3)	0.021 (2)	0.004 (2)	0.0025 (18)	0.0097 (18)
C54f	0.031 (2)	0.035 (3)	0.032 (2)	0.017 (2)	0.0175 (19)	0.0214 (19)
C55f	0.034 (2)	0.021 (2)	0.034 (2)	0.0073 (19)	0.018 (2)	0.0103 (18)
C56f	0.024 (2)	0.017 (2)	0.0229 (19)	0.0054 (17)	0.0083 (17)	0.0055 (16)
O1g	0.0289 (16)	0.0296 (18)	0.0332 (15)	0.0113 (14)	0.0157 (13)	0.0066 (14)
O1h	0.047 (2)	0.059 (2)	0.0408 (18)	0.0324 (18)	0.0293 (17)	0.0247 (16)
O1i	0.0332 (18)	0.0452 (18)	0.0278 (15)	0.0151 (15)	0.0160 (14)	0.0099 (14)
O1j	0.0352 (17)	0.051 (2)	0.0364 (16)	0.0151 (15)	0.0243 (15)	0.0118 (16)
O1k	0.0361 (17)	0.0344 (18)	0.0352 (15)	0.0133 (14)	0.0148 (14)	0.0059 (13)
O1l	0.074 (3)	0.056 (2)	0.059 (2)	0.037 (2)	0.049 (2)	0.029 (2)
O1m	0.0280 (16)	0.0276 (16)	0.0333 (16)	0.0138 (13)	0.0180 (13)	0.0112 (12)

Table S3c. Geometric parameters (Å, º) for $[Mg(OH_2)_6(C_{20}H_{14}N_2O_4)]\cdot 2.8H_2O$ (**II**).

Mg1a—O1a	2.061 (3)	C4e—C41e	1.514 (5)
Mg1a—O1a^{i}	2.061 (3)	C5e—C6e	1.394 (5)
Mg1a—O2a	2.059 (3)	C6e—H6e	0.95
Mg1a—O2a^{i}	2.059 (3)	C21e—C22e	1.397 (5)
Mg1a—O3a	2.078 (3)	C21e—C26e	1.386 (4)
Mg1a—O3a^{i}	2.078 (3)	C22e—C23e	1.385 (6)
O1a—H11a	0.840 (9)	C22e—H22e	0.95
O1a—H12a	0.840 (13)	C23e—C24e	1.381 (4)
O2a—H21a	0.84 (2)	C23e—H23e	0.95
O2a—H22a	0.840 (11)	C24e—C25e	1.382 (5)
O3a—H31a	0.84 (4)	C24e—H24e	0.95
O3a—H32a	0.840 (15)	C25e—C26e	1.389 (5)
Mg1b—O1b	2.102 (3)	C25e—H25e	0.95
Mg1b—O2b	2.058 (3)	C26e—H26e	0.95
Mg1b—O3b	2.049 (3)	C51e—C52e	1.390 (4)
Mg1b—O4b	2.042 (3)	C51e—C56e	1.392 (5)
Mg1b—O5b	2.091 (3)	C52e—C53e	1.379 (6)
Mg1b—O6b	2.064 (3)	C52e—H52e	0.95
O1b—H11b	0.84 (2)	C53e—C54e	1.380 (5)
O2b—H21b	0.840 (9)	C53e—H53e	0.95
O2b—H22b	0.84 (3)	C54e—C55e	1.386 (4)
O3b—H31b	0.84 (3)	C54e—H54e	0.95
O3b—H32b	0.840 (19)	C55e—C56e	1.391 (6)
O4b—H41b	0.840 (7)	C55e—H55e	0.95
O4b—H42b	0.84 (3)	C56e—H56e	0.95
O5b—H51b	0.84 (5)	O11f—C11f	1.254 (4)
O5b—H52b	0.840 (14)	O12f—C11f	1.285 (5)
O6b—H61b	0.840 (14)	O41f—C41f	1.258 (4)
O6b—H62b	0.84 (4)	O42f—C41f	1.271 (5)
Mg1c—O1c	2.047 (3)	N21f—C2f	1.391 (5)
Mg1c—O2c	2.033 (3)	N21f—C21f	1.405 (5)
Mg1c—O3c	2.073 (3)	N21f—H21f	0.82 (3)
Mg1c—O4c	2.051 (3)	N51f—C5f	1.390 (5)
Mg1c—O5c	2.031 (4)	N51f—C51f	1.395 (5)
Mg1c—O6c	2.071 (4)	N51f—H51f	0.84 (4)
O1c—H11c	0.84 (2)	C1f—C2f	1.423 (5)
O1c—H12c	0.84 (5)	C1f—C6f	1.391 (5)
O2c—H21c	0.840 (16)	C1f—C11f	1.500 (5)
O2c—H22c	0.840 (11)	C2f—C3f	1.396 (5)
O3c—H31c	0.840 (15)	C3f—C4f	1.385 (5)
O4c—H41c	0.840 (12)	C3f—H3f	0.95
O4c—H42c	0.840 (16)	C4f—C5f	1.415 (5)
O5c—H51c	0.84 (4)	C4f—C41f	1.509 (5)
O5c—H52c	0.84 (5)	C5f—C6f	1.397 (5)
O6c—H61c	0.84 (4)	C6f—H6f	0.95
O6c—H62c	0.84 (3)	C21f—C22f	1.394 (5)
O11d—C11d	1.260 (4)	C21f—C26f	1.394 (4)
O12d—C11d	1.265 (5)	C22f—C23f	1.399 (6)
N21d—C2d	1.395 (5)	C22f—H22f	0.95
N21d—C21d	1.406 (5)	C23f—C24f	1.376 (4)
N21d—H21d	0.85 (4)	C23f—H23f	0.95
C1d—C2d^{ii}	1.420 (6)	C24f—C25f	1.385 (5)
C1d—C3d	1.389 (5)	C24f—H24f	0.95
C1d—C11d	1.512 (6)	C25f—C26f	1.384 (6)

C2d—C3d	1.394 (5)	C25f—H25f	0.95
C3d—H3d	0.95	C26f—H26f	0.95
C21d—C22d	1.405 (5)	C51f—C52f	1.392 (4)
C21d—C26d	1.389 (4)	C51f—C56f	1.392 (5)
C22d—C23d	1.380 (6)	C52f—C53f	1.379 (6)
C22d—H22d	0.95	C52f—H52f	0.95
C23d—C24d	1.382 (4)	C53f—C54f	1.376 (5)
C23d—H23d	0.95	C53f—H53f	0.95
C24d—C25d	1.380 (5)	C54f—C55f	1.381 (4)
C24d—H24d	0.95	C54f—H54f	0.95
C25d—C26d	1.395 (6)	C55f—C56f	1.379 (6)
C25d—H25d	0.95	C55f—H55f	0.95
C26d—H26d	0.95	C56f—H56f	0.95
O11e—C11e	1.259 (4)	O1g—H11g	0.84 (5)
O12e—C11e	1.274 (5)	O1g—H12g	0.840 (10)
O41e—C41e	1.248 (4)	O1h—H11h	0.84 (5)
O42e—C41e	1.283 (5)	O1h—H12h	0.84 (4)
N21e—C2e	1.401 (5)	O1i—H11i	0.84 (5)
N21e—C21e	1.395 (5)	O1i—H12i	0.84 (8)
N21e—H21e	0.80 (3)	O1j—H12j	0.84 (8)
N51e—C5e	1.393 (5)	O1k—H12k	0.84 (3)
N51e—C51e	1.407 (5)	O1l—H12l	0.84 (3)
N51e—H51e	0.82 (4)	O1m—H11m	0.84 (5)
C1e—C2e	1.409 (5)	O1m—H12m	0.84 (4)
C1e—C6e	1.393 (5)	H12b—O1b	0.840 (11)
C1e—C11e	1.504 (5)	H32c—O3c	0.84 (3)
C2e—C3e	1.403 (5)	H11j—O1j	0.94 (6)
C3e—C4e	1.381 (5)	H11k—O1k	0.84 (7)
C3e—H3e	0.95	H11l—O1l	0.84 (5)
C4e—C5e	1.418 (5)		

O1a—Mg1a—O1a^{i}	180.0	N21e—C2e—C1e	123.2 (3)
O1a—Mg1a—O2a	90.46 (11)	N21e—C2e—C3e	119.7 (3)
O1a—Mg1a—O2a^{i}	89.54 (11)	C1e—C2e—C3e	117.1 (3)
O1a—Mg1a—O3a	88.24 (12)	C2e—C3e—C4e	123.7 (3)
O1a—Mg1a—O3a^{i}	91.76 (12)	C2e—C3e—H3e	118.14
O1a^{i}—Mg1a—O2a	89.54 (11)	C4e—C3e—H3e	118.14
O1a^{i}—Mg1a—O2a^{i}	90.46 (11)	C3e—C4e—C5e	119.2 (3)
O1a^{i}—Mg1a—O3a	91.76 (12)	C3e—C4e—C41e	118.3 (3)
O1a^{i}—Mg1a—O3a^{i}	88.24 (12)	C5e—C4e—C41e	122.5 (3)
O2a—Mg1a—O2a^{i}	180.0	N51e—C5e—C4e	122.3 (3)
O2a—Mg1a—O3a	90.00 (11)	N51e—C5e—C6e	120.5 (3)
O2a—Mg1a—O3a^{i}	90.00 (11)	C4e—C5e—C6e	117.2 (3)
O2a^{i}—Mg1a—O3a	90.00 (11)	C1e—C6e—C5e	123.5 (3)
O2a^{i}—Mg1a—O3a^{i}	90.00 (11)	C1e—C6e—H6e	118.23
O3a—Mg1a—O3a^{i}	180.0	C5e—C6e—H6e	118.23
Mg1a—O1a—H11a	111 (2)	O11e—C11e—O12e	123.0 (3)
Mg1a—O1a—H12a	115 (2)	O11e—C11e—C1e	119.6 (3)
H11a—O1a—H12a	113 (3)	O12e—C11e—C1e	117.3 (3)
Mg1a—O2a—H21a	116 (3)	O41e—C41e—O42e	123.4 (3)
Mg1a—O2a—H22a	124 (3)	O41e—C41e—C4e	119.7 (4)
H21a—O2a—H22a	113 (3)	O42e—C41e—C4e	116.9 (3)
Mg1a—O3a—H31a	117.9 (18)	N21e—C21e—C22e	119.2 (2)
Mg1a—O3a—H32a	111 (2)	N21e—C21e—C26e	122.4 (3)
H31a—O3a—H32a	113 (4)	C22e—C21e—C26e	118.3 (3)
O1b—Mg1b—O2b	87.18 (13)	C21e—C22e—C23e	120.8 (3)
O1b—Mg1b—O3b	177.55 (16)	C21e—C22e—H22e	119.62

O1b—Mg1b—O4b	91.43 (13)	C23e—C22e—H22e	119.62
O1b—Mg1b—O5b	88.13 (12)	C22e—C23e—C24e	120.7 (3)
O1b—Mg1b—O6b	91.12 (12)	C22e—C23e—H23e	119.66
O2b—Mg1b—O3b	90.73 (12)	C24e—C23e—H23e	119.66
O2b—Mg1b—O4b	178.10 (12)	C23e—C24e—C25e	118.8 (4)
O2b—Mg1b—O5b	89.34 (13)	C23e—C24e—H24e	120.59
O2b—Mg1b—O6b	90.91 (12)	C25e—C24e—H24e	120.59
O3b—Mg1b—O4b	90.62 (13)	C24e—C25e—C26e	120.9 (3)
O3b—Mg1b—O5b	90.56 (12)	C24e—C25e—H25e	119.53
O3b—Mg1b—O6b	90.20 (12)	C26e—C25e—H25e	119.53
O4b—Mg1b—O5b	89.31 (12)	C21e—C26e—C25e	120.5 (3)
O4b—Mg1b—O6b	90.41 (13)	C21e—C26e—H26e	119.75
O5b—Mg1b—O6b	179.19 (12)	C25e—C26e—H26e	119.75
Mg1b—O1b—H11b	129 (4)	N51e—C51e—C52e	122.8 (3)
Mg1b—O2b—H21b	116 (3)	N51e—C51e—C56e	119.3 (2)
Mg1b—O2b—H22b	116 (3)	C52e—C51e—C56e	117.8 (3)
H21b—O2b—H22b	113 (3)	C51e—C52e—C53e	121.1 (3)
Mg1b—O3b—H31b	123 (3)	C51e—C52e—H52e	119.45
Mg1b—O3b—H32b	117 (2)	C53e—C52e—H52e	119.45
H31b—O3b—H32b	113 (3)	C52e—C53e—C54e	121.1 (3)
Mg1b—O4b—H41b	119 (3)	C52e—C53e—H53e	119.45
Mg1b—O4b—H42b	117 (3)	C54e—C53e—H53e	119.45
H41b—O4b—H42b	113 (3)	C53e—C54e—C55e	118.5 (4)
Mg1b—O5b—H51b	122 (2)	C53e—C54e—H54e	120.73
Mg1b—O5b—H52b	110 (2)	C55e—C54e—H54e	120.73
H51b—O5b—H52b	113 (4)	C54e—C55e—C56e	120.6 (3)
Mg1b—O6b—H61b	114.6 (18)	C54e—C55e—H55e	119.71
Mg1b—O6b—H62b	123.1 (17)	C56e—C55e—H55e	119.71
H61b—O6b—H62b	113 (3)	C51e—C56e—C55e	120.9 (3)
O1c—Mg1c—O2c	91.08 (12)	C51e—C56e—H56e	119.55
O1c—Mg1c—O3c	175.48 (16)	C55e—C56e—H56e	119.55
O1c—Mg1c—O4c	90.84 (11)	C2f—N21f—C21f	126.2 (3)
O1c—Mg1c—O5c	92.74 (14)	C2f—N21f—H21f	117 (3)
O1c—Mg1c—O6c	89.53 (13)	C21f—N21f—H21f	116 (3)
O2c—Mg1c—O3c	91.60 (11)	C5f—N51f—C51f	127.2 (3)
O2c—Mg1c—O4c	178.03 (11)	C5f—N51f—H51f	113 (3)
O2c—Mg1c—O5c	89.34 (15)	C51f—N51f—H51f	118 (3)
O2c—Mg1c—O6c	88.45 (15)	C2f—C1f—C6f	119.0 (3)
O3c—Mg1c—O4c	86.45 (11)	C2f—C1f—C11f	122.9 (3)
O3c—Mg1c—O5c	90.93 (13)	C6f—C1f—C11f	118.1 (3)
O3c—Mg1c—O6c	86.90 (13)	N21f—C2f—C1f	122.8 (3)
O4c—Mg1c—O5c	90.95 (15)	N21f—C2f—C3f	120.2 (3)
O4c—Mg1c—O6c	91.18 (15)	C1f—C2f—C3f	117.0 (3)
O5c—Mg1c—O6c	176.86 (13)	C2f—C3f—C4f	123.8 (3)
Mg1c—O1c—H11c	117 (3)	C2f—C3f—H3f	118.1
Mg1c—O1c—H12c	121 (2)	C4f—C3f—H3f	118.1
H11c—O1c—H12c	113 (3)	C3f—C4f—C5f	119.4 (3)
Mg1c—O2c—H21c	120 (2)	C3f—C4f—C41f	116.8 (3)
Mg1c—O2c—H22c	126 (2)	C5f—C4f—C41f	123.7 (3)
H21c—O2c—H22c	113 (3)	N51f—C5f—C4f	121.9 (3)
Mg1c—O3c—H31c	120 (2)	N51f—C5f—C6f	121.1 (3)
Mg1c—O4c—H41c	117 (2)	C4f—C5f—C6f	117.0 (3)
Mg1c—O4c—H42c	120 (2)	C1f—C6f—C5f	123.7 (4)
H41c—O4c—H42c	113 (3)	C1f—C6f—H6f	118.13
Mg1c—O5c—H51c	121 (3)	C5f—C6f—H6f	118.13
Mg1c—O5c—H52c	125 (4)	O11f—C11f—O12f	121.8 (3)
H51c—O5c—H52c	113 (5)	O11f—C11f—C1f	119.9 (4)

Mg1c—O6c—H61c	125 (3)	O12f—C11f—C1f	118.3 (3)
Mg1c—O6c—H62c	119 (4)	O41f—C41f—O42f	122.6 (3)
H61c—O6c—H62c	113 (4)	O41f—C41f—C4f	120.0 (3)
C2d—N21d—C21d	126.9 (3)	O42f—C41f—C4f	117.4 (3)
C2d—N21d—H21d	117 (3)	N21f—C21f—C22f	119.3 (2)
C21d—N21d—H21d	113 (3)	N21f—C21f—C26f	122.6 (3)
C2d^{ii}—C1d—C3d	118.9 (3)	C22f—C21f—C26f	118.0 (3)
C2d^{ii}—C1d—C11d	123.2 (3)	C21f—C22f—C23f	120.5 (3)
C3d—C1d—C11d	117.9 (3)	C21f—C22f—H22f	119.73
N21d—C2d—C1d^{ii}	121.8 (3)	C23f—C22f—H22f	119.73
N21d—C2d—C3d	120.7 (4)	C22f—C23f—C24f	120.5 (3)
C1d^{ii}—C2d—C3d	117.5 (3)	C22f—C23f—H23f	119.74
C1d—C3d—C2d	123.6 (4)	C24f—C23f—H23f	119.73
C1d—C3d—H3d	118.2	C23f—C24f—C25f	119.4 (4)
C2d—C3d—H3d	118.2	C23f—C24f—H24f	120.32
O11d—C11d—O12d	122.9 (4)	C25f—C24f—H24f	120.32
O11d—C11d—C1d	119.6 (4)	C24f—C25f—C26f	120.3 (3)
O12d—C11d—C1d	117.5 (3)	C24f—C25f—H25f	119.83
N21d—C21d—C22d	118.1 (2)	C26f—C25f—H25f	119.83
N21d—C21d—C26d	123.7 (3)	C21f—C26f—C25f	121.2 (3)
C22d—C21d—C26d	118.0 (3)	C21f—C26f—H26f	119.4
C21d—C22d—C23d	120.7 (3)	C25f—C26f—H26f	119.4
C21d—C22d—H22d	119.64	N51f—C51f—C52f	123.2 (3)
C23d—C22d—H22d	119.64	N51f—C51f—C56f	118.7 (3)
C22d—C23d—C24d	121.0 (3)	C52f—C51f—C56f	118.0 (3)
C22d—C23d—H23d	119.52	C51f—C52f—C53f	120.7 (3)
C24d—C23d—H23d	119.52	C51f—C52f—H52f	119.65
C23d—C24d—C25d	118.9 (4)	C53f—C52f—H52f	119.65
C23d—C24d—H24d	120.57	C52f—C53f—C54f	121.0 (3)
C25d—C24d—H24d	120.57	C52f—C53f—H53f	119.49
C24d—C25d—C26d	120.9 (3)	C54f—C53f—H53f	119.49
C24d—C25d—H25d	119.56	C53f—C54f—C55f	118.7 (4)
C26d—C25d—H25d	119.56	C53f—C54f—H54f	120.66
C21d—C26d—C25d	120.5 (3)	C55f—C54f—H54f	120.66
C21d—C26d—H26d	119.74	C54f—C55f—C56f	120.9 (3)
C25d—C26d—H26d	119.74	C54f—C55f—H55f	119.56
C2e—N21e—C21e	126.5 (3)	C56f—C55f—H55f	119.56
C2e—N21e—H21e	113 (2)	C51f—C56f—C55f	120.7 (3)
C21e—N21e—H21e	118 (3)	C51f—C56f—H56f	119.64
C5e—N51e—C51e	126.2 (3)	C55f—C56f—H56f	119.64
C5e—N51e—H51e	117 (3)	H11g—O1g—H12g	113 (4)
C51e—N51e—H51e	114 (3)	H11h—O1h—H12h	113 (5)
C2e—C1e—C6e	119.2 (3)	H11i—O1i—H12i	113 (5)
C2e—C1e—C11e	123.1 (3)	H11m—O1m—H12m	113 (5)
C6e—C1e—C11e	117.6 (3)		

Symmetry codes: (i) -x+1, -y, -z+2; (ii) -x+1, -y+1, -z+1.

Table S3d. Hydrogen-bond geometry (Å, º) for $[Mg(OH_2)_6(C_{20}H_{14}N_2O_4)]\cdot 2.8H_2O$ (**II**).

D—H···A	D—H	H···A	D···A	D—H···A
C3*d*—H3*d*···O12*d*	0.95	2.40	2.753 (5)	101.74
N21*d*—H21*d*···O11*d*^{ii}	0.85 (4)	2.06 (5)	2.698 (5)	132 (3)
C3*e*—H3*e*···O42*e*	0.95	2.41	2.762 (5)	101.75
C6*e*—H6*e*···O12*e*	0.95	2.39	2.746 (5)	101.75
N21*e*—H21*e*···O11*e*	0.80 (3)	2.09 (4)	2.720 (4)	136 (3)
N51*e*—H51*e*···O41*e*	0.82 (4)	2.08 (4)	2.702 (4)	133 (3)
C3*f*—H3*f*···O42*f*	0.95	2.35	2.722 (4)	102.79
C6*f*—H6*f*···O12*f*	0.95	2.41	2.768 (4)	102.07
N21*f*—H21*f*···O11*f*	0.82 (3)	2.11 (4)	2.708 (4)	130 (4)
N51*f*—H51*f*···O41*f*	0.84 (4)	2.06 (4)	2.714 (4)	134 (3)
O1*a*—H11*a*···O12*e*^{i}	0.840 (9)	1.922 (14)	2.745 (3)	166 (3)
O1*a*—H12*a*···O41*f*^{iii}	0.840 (13)	1.895 (15)	2.729 (3)	172 (4)
O2*a*—H21*a*···O12*e*^{i}	0.84 (2)	2.07 (3)	2.851 (4)	154 (3)
O2*a*—H22*a*···O1*i*^{iv}	0.840 (11)	1.940 (18)	2.769 (4)	169 (4)
O3*a*—H32*a*···O42*f*^{v}	0.840 (15)	1.884 (15)	2.724 (3)	178 (5)
O1*b*—H11*b*···O11*f*	0.84 (2)	1.87 (3)	2.690 (4)	163 (5)
O1*b*—H12*b*···O12*d*	0.840 (11)	2.25 (2)	3.071 (4)	166 (5)
O2*b*—H21*b*···O1*m*	0.840 (9)	1.908 (16)	2.719 (3)	162 (3)
O2*b*—H22*b*···O12*d*	0.84 (3)	1.89 (3)	2.720 (4)	169 (4)
O3*b*—H31*b*···O1*l*	0.84 (3)	1.92 (3)	2.754 (6)	174 (2)
O3*b*—H32*b*···O41*e*^{vi}	0.840 (19)	1.88 (2)	2.718 (4)	174 (3)
O4*b*—H41*b*···O1*g*	0.840 (7)	1.979 (13)	2.803 (3)	166 (4)
O4*b*—H42*b*···O12*f*^{iv}	0.84 (3)	1.95 (3)	2.771 (4)	166 (2)
O5*b*—H52*b*···O12*f*	0.840 (14)	1.886 (14)	2.716 (3)	170 (5)
O6*b*—H61*b*···O42*e*^{vi}	0.840 (14)	1.991 (14)	2.806 (3)	163 (3)
O1*c*—H11*c*···O12*d*^{vii}	0.84 (2)	1.85 (2)	2.689 (4)	176 (4)
O1*c*—H12*c*···O1*k*	0.84 (5)	2.16 (4)	2.951 (5)	157 (3)
O2*c*—H21*c*···O11*e*^{viii}	0.840 (16)	1.905 (16)	2.741 (3)	173 (3)
O2*c*—H22*c*···O42*e*^{ii}	0.840 (11)	1.862 (10)	2.694 (4)	171 (3)
O3*c*—H31*c*···O12*e*^{viii}	0.840 (15)	1.831 (17)	2.668 (4)	175 (3)
O3*c*—H32*c*···O42*f*^{vi}	0.84 (3)	1.98 (3)	2.817 (4)	174 (3)
O4*c*—H41*c*···O11*d*^{vii}	0.840 (12)	1.859 (14)	2.695 (3)	173 (3)
O4*c*—H42*c*···O42*f*^{vi}	0.840 (16)	2.049 (16)	2.850 (3)	159 (3)
O5*c*—H51*c*···O1*j*	0.84 (4)	1.88 (4)	2.709 (5)	174 (3)
O6*c*—H62*c*···O1*m*^{vii}	0.84 (3)	1.84 (3)	2.678 (4)	173 (5)
O1*g*—H11*g*···O12*f*	0.84 (5)	2.00 (5)	2.822 (5)	165 (4)
O1*g*—H12*g*···O5*b*^{iv}	0.840 (10)	2.17 (3)	2.915 (4)	148 (5)
O1*h*—H11*h*···O11*e*	0.84 (5)	2.02 (5)	2.845 (5)	169 (5)
O1*h*—H12*h*···O3*c*^{ix}	0.84 (4)	2.33 (4)	2.934 (5)	129 (4)
O1*i*—H11*i*···O1*g*	0.84 (5)	2.00 (5)	2.808 (5)	162 (4)
O1*i*—H12*i*···O41*f*^{vi}	0.84 (8)	2.21 (8)	3.049 (5)	176 (7)
O1*j*—H11*j*···O1*i*	0.94 (6)	1.92 (5)	2.835 (4)	163 (7)
O1*j*—H12*j*···O1*b*	0.84 (8)	1.94 (8)	2.776 (5)	171 (6)
O1*k*—H11*k*···O11*d*	0.84 (7)	2.30 (8)	3.121 (5)	164 (7)
O1*k*—H12*k*···O1*j*^{vii}	0.84 (3)	2.02 (3)	2.855 (4)	173 (6)
O1*l*—H12*l*···O1*h*	0.84 (3)	2.01 (3)	2.846 (5)	172 (6)
O1*m*—H11*m*···O42*e*^{vi}	0.84 (5)	1.94 (6)	2.755 (5)	165 (4)
O1*m*—H12*m*···O1*h*	0.84 (4)	1.88 (5)	2.704 (5)	167 (4)

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

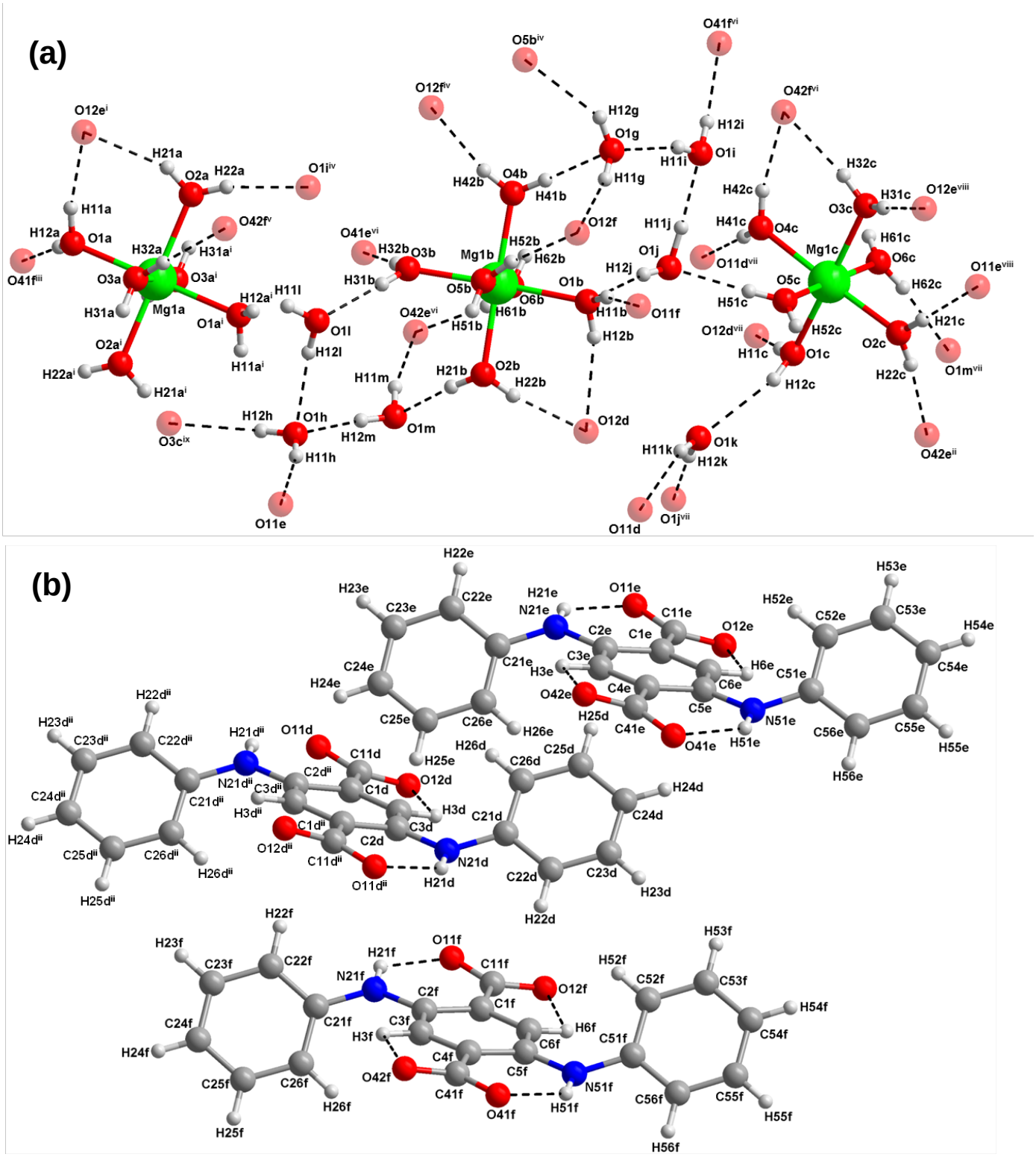

Figure S3b. Representation of hydrogen bonds (dashed lines) for $[Mg(OH_2)_6(C_{20}H_{14}N_2O_4)]\cdot 2.8H_2O$ (**II**) focused on both the Mg^{2+} (a) and the 2,5-(dianilino)terephthalate dianion (b) environments.
Symmetry codes: (i) -x+1, -y, -z+2; (ii) -x+1, -y+1, -z+1; (iii) x+1, y, z+1; (iv) -x+1, -y, -z+1; (v) -x, -y, -z+1; (vi) x+1, y, z; (vii) -x+2, -y+1, -z+1; (viii) x, y, z-1; (ix) x, y, z+1.

4. DFT calculations

Table S4a. Experimental, DFT optimized fractional atomic coordinates, and atomic displacement (in Å) during DFT optimization for $[(Li(OH_2)_3)_2(C_{20}H_{14}N_2O_4)]\cdot 2H_2O$ (**Ia**, form α).

	DRX			DFT			Displacement (Ang.)
Atom	x	y	z	x	y	z	
O11a	0.37413 (18)	0.75585 (17)	0.23134 (13)	0.37672	0.75831	0.23141	0.03
O12a	0.58286 (18)	0.58030 (17)	0.19178 (13)	0.58368	0.57915	0.18889	0.03
N21a	0.7710 (2)	0.2653 (2)	0.56877 (17)	0.77404	0.26885	0.57246	0.04
C1a	0.4833 (3)	0.5700 (2)	0.38413 (19)	0.48347	0.56865	0.38281	0.02
C2a	0.6312 (3)	0.3790 (2)	0.5343 (2)	0.63382	0.38053	0.53638	0.03
C3a	0.6100 (3)	0.4505 (2)	0.4207 (2)	0.61185	0.45002	0.42089	0.02
C11a	0.4786 (3)	0.6406 (2)	0.2611 (2)	0.47980	0.64008	0.26072	0.01
C21a	0.8441 (3)	0.1879 (3)	0.4645 (2)	0.84676	0.19024	0.46903	0.05
C22a	0.7453 (3)	0.0571 (3)	0.3722 (2)	0.74409	0.05923	0.37516	0.04
C23a	0.8177 (3)	0.9859 (3)	0.2733 (2)	0.81408	0.98844	0.27310	0.04
C24a	0.9875 (3)	0.0447 (3)	0.2656 (2)	0.98507	0.04829	0.26381	0.04
C25a	0.0854 (3)	0.1755 (3)	0.3564 (2)	0.08700	0.17969	0.35688	0.04
C26a	0.0131 (3)	0.2469 (3)	0.4568 (2)	0.01748	0.25038	0.45946	0.04
H21a	0.734 (3)	0.201 (3)	0.618 (3)	0.73920	0.19444	0.63197	0.14
H22a	0.628003	0.016271	0.376832	0.60884	0.01412	0.38077	0.16
H23a	0.750022	0.895643	0.209919	0.73400	0.88648	0.20021	0.14
H24a	0.036885	0.994613	0.19741	0.03853	0.99290	0.18364	0.15
H25a	0.201797	0.217037	0.350789	0.22059	0.22681	0.34977	0.17
H26a	0.081053	0.33683	0.520383	0.09548	0.35319	0.53262	0.18
H3a	0.686019	0.415904	0.365122	0.69909	0.41137	0.35721	0.15
O1b	0.4557 (2)	0.72309 (19)	0.97006 (18)	0.45825	0.72307	0.97070	0.02
O2b	0.2831 (3)	0.0645 (2)	0.07668 (17)	0.27908	0.07183	0.07344	0.08
O3b	0.0202 (2)	0.7220 (2)	0.98574 (18)	0.02003	0.71952	0.98584	0.02
Li1b	0.2784 (5)	0.8319 (4)	0.0588 (4)	0.27683	0.83779	0.05694	0.06
H11b	0.507 (4)	0.672 (4)	0.041 (3)	0.51769	0.66987	0.05143	0.11
H12b	0.430 (3)	0.644 (4)	0.899 (3)	0.43207	0.63040	0.89582	0.14
H21b	0.387 (4)	0.125 (4)	0.071 (3)	0.38164	0.13935	0.06101	0.16
H22b	0.187 (4)	0.119 (4)	0.060 (3)	0.17079	0.14242	0.05871	0.23
H31b	0.998 (3)	0.675 (3)	0.054 (3)	0.99322	0.66741	0.05773	0.10
H32b	0.016 (4)	0.638 (4)	0.921 (3)	0.01879	0.62754	0.91384	0.11
O1c	0.9540 (3)	0.5667 (2)	0.18607 (17)	0.95388	0.56797	0.18337	0.03
H11c	0.037 (4)	0.609 (4)	0.257 (3)	0.04443	0.61783	0.27118	0.15
H12c	0.837 (4)	0.570 (4)	0.200 (3)	0.82659	0.57676	0.19463	0.12

Table S4b. Experimental, DFT optimized fractional atomic coordinates, and atomic displacement (in Å) during DFT optimization for $[(Li(OH_2)_4)_2(C_{20}H_{14}N_2O_4)]$ (**Ib**, form β).

	DRX			DFT			Displacement (Ang.)
Atom	x	y	z	x	y	z	
O11a	0.20752 (13)	0.5768 (3)	0.04897 (11)	0.20843	0.57654	0.05008	0.02
O12a	0.29928 (12)	0.8726 (3)	0.01691 (9)	0.30165	0.87257	0.01475	0.05
N21a	0.00787 (17)	0.3872 (3)	0.91189 (12)	0.00523	0.38227	0.90863	0.07
C1a	0.09908 (19)	0.8856 (4)	0.01788 (13)	0.10061	0.88698	0.01768	0.02
C2a	0.00377 (19)	0.1948 (4)	0.95493 (13)	0.00278	0.19386	0.95328	0.03
C3a	0.1005 (2)	0.0790 (4)	0.97546 (13)	0.10026	0.07828	0.97343	0.03
C11a	0.20846 (19)	0.7688 (4)	0.02927 (13)	0.20955	0.77103	0.02895	0.02
C21a	0.08091 (19)	0.4489 (4)	0.85043 (14)	0.07990	0.44719	0.84943	0.02
C22a	0.0739 (2)	0.6586 (4)	0.82151 (15)	0.07209	0.65890	0.82035	0.03
C23a	0.1410 (2)	0.7272 (5)	0.75842 (15)	0.14315	0.73267	0.75970	0.05
C24a	0.2187 (2)	0.5929 (5)	0.72366 (15)	0.22415	0.59920	0.72612	0.09
C25a	0.2246 (2)	0.3852 (5)	0.75105 (16)	0.23026	0.38795	0.75298	0.08
C26a	0.1574 (2)	0.3130 (4)	0.81332 (15)	0.15950	0.31228	0.81360	0.03
H3a	0.170585	0.134886	0.959747	0.18061	0.13962	0.95487	0.15
H21a	0.944 (2)	0.477 (4)	0.9174 (16)	0.93331	0.46936	0.91478	0.14
H22a	0.022501	0.754389	0.845518	0.00947	0.76464	0.84593	0.17
H23a	0.133754	0.868887	0.738446	0.13565	0.89647	0.73824	0.17
H24a	0.26697	0.642761	0.681889	0.28066	0.65801	0.67950	0.20
H25a	0.27592	0.290219	0.726529	0.29148	0.27983	0.72722	0.20
H26a	0.163024	0.169256	0.83123	0.16463	0.14612	0.83159	0.15
O1b	0.48808 (16)	0.7008 (3)	0.09258 (11)	0.48861	0.69633	0.09247	0.03
O2b	0.37169 (15)	0.2848 (3)	0.05189 (11)	0.37291	0.28740	0.04635	0.09
O3b	0.61718 (16)	0.2613 (3)	0.13076 (12)	0.61470	0.25186	0.13403	0.09
O4b	0.45602 (17)	0.4400 (4)	0.25620 (12)	0.45398	0.43026	0.25975	0.09
Li1b	0.4753 (3)	0.4094 (7)	0.1362 (3)	0.47291	0.40592	0.13869	0.05
H11b	0.534 (2)	0.707 (5)	0.053 (2)	0.54429	0.69943	0.04749	0.16
H12b	0.420 (3)	0.758 (6)	0.067 (2)	0.41921	0.75719	0.06550	0.02
H21b	0.320 (3)	0.382 (6)	0.049 (2)	0.31033	0.39438	0.04403	0.15
H22b	0.341 (3)	0.149 (6)	0.042 (2)	0.33858	0.14427	0.03993	0.06
H31b	0.649 (3)	0.210 (6)	0.080 (2)	0.64612	0.20089	0.08062	0.08
H32b	0.669 (2)	0.318 (5)	0.1589 (19)	0.67692	0.31793	0.16612	0.17
H41b	0.421 (3)	0.541 (5)	0.286 (2)	0.42429	0.55014	0.29242	0.12
H42b	0.477 (3)	0.348 (6)	0.293 (2)	0.47474	0.32777	0.30430	0.22

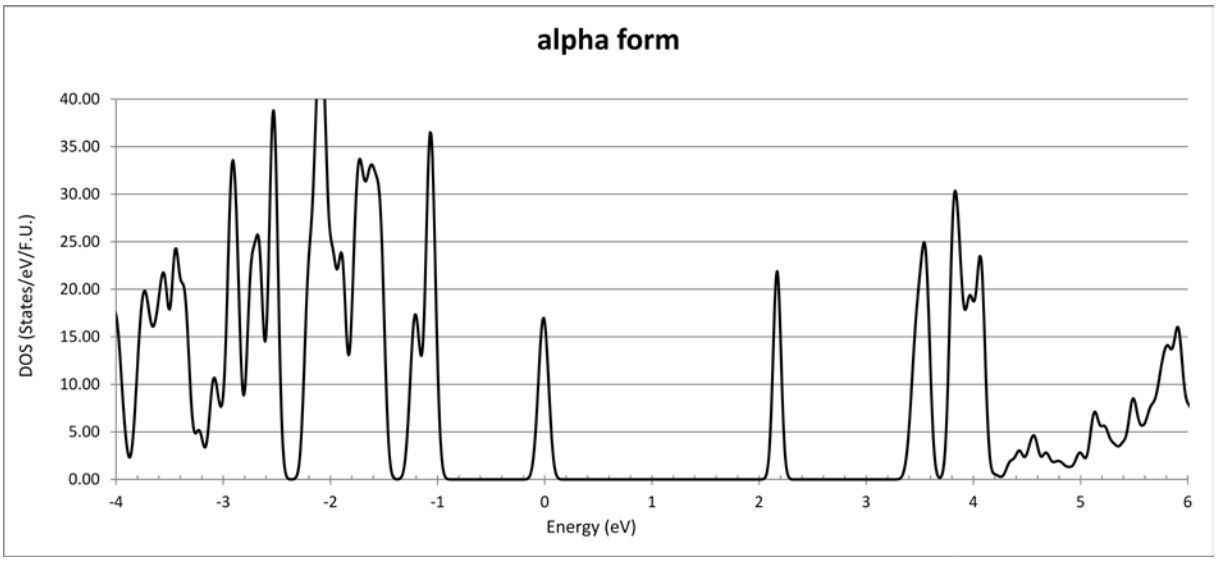

Figure S4a. Total Density of states (DOS) for compound **Ia** (form α) (top) and compound **Ib** (form β) (bottom).

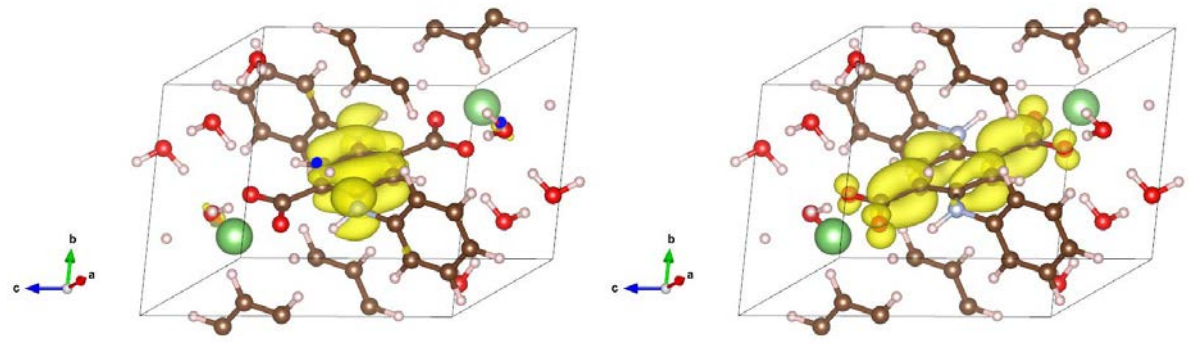

Figure S4b. Isosurface of the partial charge density calculated for the HOMO (left) and LUMO (right) for compound **Ia** (form α).

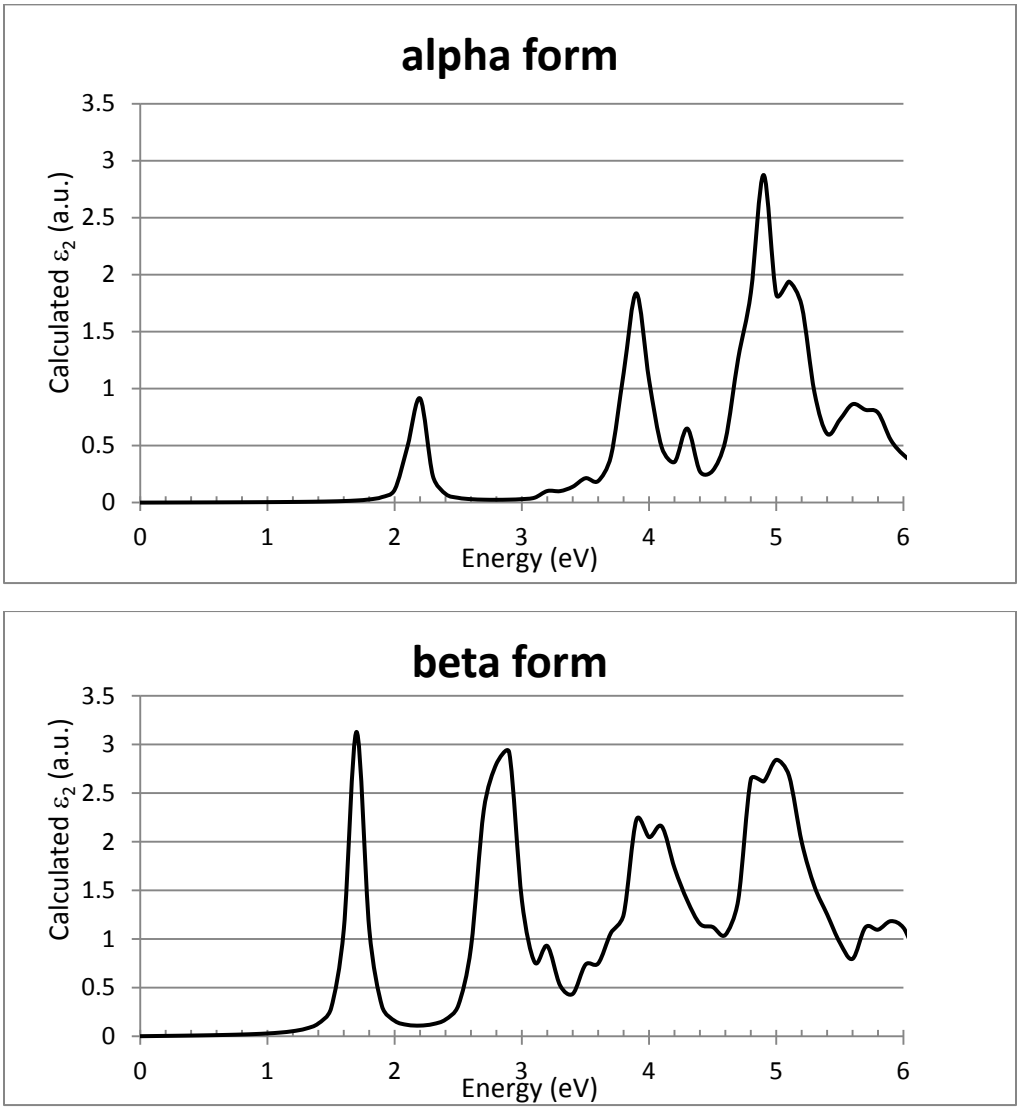

Figure S4c. Imaginary part of the calculated dielectric constant for compound **Ia** (form α) (top) and compound **Ib** (form β) (bottom).