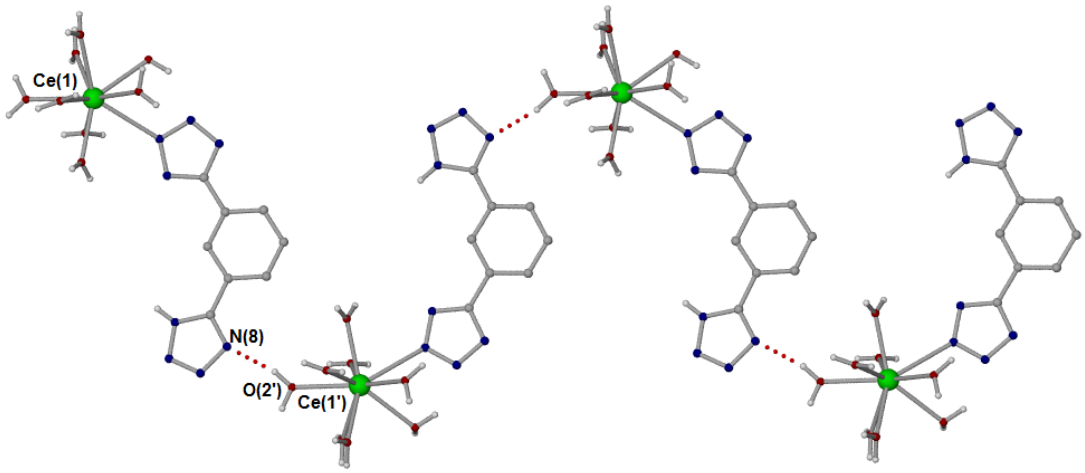

Figure S1 The 1D H-bonded $[Ce(H_2O)_8(m\text{-BDTH})]^{2+}$ cationic chain parallel to *a*0*c* plane. Lattice water molecules are omitted for clarity (symmetry operation -1/2 + *x*,1/2 – *y*, *z* – ½)

Table S1 Parameters for hydrogen bonding in **1**.

N5-H5 ··· O12	0.85(5)	1.86(5)	2.673(5)	162(4)
O1-H11 ··· O13	0.87(4)	1.99(5)	2.716(5)	140(5)
O1-H12 ···N14	0.83(5)	2.02(5)	2.847(5)	174(6)[b]
O2-H21 ···N8	0.84(5)	2.00(6)	2.819(5)	165(5)[d]
O2-H22 ···O20	0.86(4)	1.96(4)	2.811(5)	177(7)[a]
O3-H31 ···O14	0.84(4)	1.92(4)	2.748(5)	168(5)
O3-H32 ···O11	0.84(4)	1.89(5)	2.721(5)	176(6)
O4-H41 ··· N9	0.84(5)	1.99(5)	2.825(5)	170(5)[e]
O4-H42 ··· O6	0.85(4)	1.92(4)	2.770(4)	176(6)[a]
O5-H51 ··· N10	0.87(4)	2.23(5)	3.072(5)	162(5)[f]
O5-H52 ··· O22A	0.87(3)	1.96(4)	2.796(9)	162(5)
O5-H52 ··· O22B	0.87(3)	2.16(3)	3.022(8)	170(5)
O6-H61 ··· O16	0.87(5)	1.88(5)	2.747(5)	175(4)
O6-H62 ··· N2	0.86(5)	1.96(5)	2.710(5)	145(4)
O7-H71 ··· O20	0.87(5)	1.95(5)	2.821(5)	174(5)[g]
O7-H72 ··· N10	0.86(4)	2.04(4)	2.888(5)	170(4)[f]
O8-H81 ··· O17	0.83(4)	1.92(3)	2.736(5)	169(5)
O8-H82 ··· N11	0.86(5)	2.08(5)	2.927(6)	174(6)[d]
O11-H111··· N4	0.85(5)	1.87(5)	2.702(5)	171(4)
O11-H112 ··· O15	0.83(4)	1.95(4)	2.751(5)	164(5)[g]
O12-H121 ··· O19	0.83(5)	1.89(5)	2.724(5)	177(7)[d]
O12-H122 ··· O11	0.85(4)	1.83(4)	2.673(4)	171(6)
O13-H132 ··· O22A	0.85(5)	2.41(6)	2.854(10)	113(5)
O14-H142 ··· N13	0.84(5)	1.90(5)	2.731(5)	173(4)[b]
O15-H151 ··· N12	0.85(5)	1.91(5)	2.743(5)	168(5)[d]
O16-H161 ··· O17	0.86(5)	1.91(4)	2.741(5)	161(6)
O17-H171 ··· O19	0.85(5)	1.97(5)	2.799(5)	165(5)[g]
O17-H172 ··· N16	0.85(6)	1.94(6)	2.785(5)	173(4)

O18-H181 ··· N15	0.87(5)	1.93(5)	2.794(5)	171(6)[b]
O19-H191 ··· O15	0.85(5)	1.88(5)	2.728(5)	174(5)
O19-H192 ··· O21	0.86(5)	1.88(6)	2.732(5)	170(6)
O20-H201 ··· O18	0.87(3)	1.85(4)	2.707(6)	168(4)[a]
O20-H202 ··· O21	0.86(5)	2.31(5)	3.038(5)	143(5)
O21-H211 ··· N1	0.85(6)	2.01(6)	2.843(5)	166(6)
O21-H212 ··· O22B	0.82(5)	2.10(6)	2.774(10)	139(5)[a]

Symmetry operation
[a] 1-x,1-y,1-z
[b] x,y,1+z
[d] -1/2+x,1/2-y,1/2+z
[e] 1/2+x,1/2-y,1/2+z
[f] 1/2-x,1/2+y,1/2-z
[g] -1+x,y,z

Table S2 Parameters for hydrogen bonding in **2**.

N5-H5 ··· O12	0.84(5)	1.85(5)	2.668(5)	166(4)
O1-H11 ··· O13	0.86(4)	1.87(5)	2.719(5)	169(5)[a]
O1-H12 ···N14	0.86(5)	1.99(5)	2.845(5)	176(6)[b]
O2-H21 ···N8	0.83(5)	2.00(6)	2.816(5)	167(5)[c]
O2-H22 ···O20	0.86(4)	1.95(4)	2.810(5)	178(7)[d]
O3-H31 ···O14	0.86(4)	1.91(4)	2.758(5)	174(5)[c]
O3-H32 ···O11	0.80(4)	1.93(5)	2.725(5)	174(6)
O4-H41 ··· N9	0.86(5)	1.99(5)	2.833 (5)	169(5)[a]
O4-H42 ··· O6	0.87(4)	1.90(4)	2.776(4)	175(6)[e]
O5-H51 ··· N10	0.84(4)	2.29(5)	3.071(5)	155(5)[f]
O5-H52 ··· O22A	0.85(3)	1.96(4)	2.795(9)	166(5)[g]
O5-H52 ··· O22B	0.85(3)	2.18(3)	3.021(8)	169(5)[g]
O6-H61 ··· O16	0.84(5)	1.91(5)	2.743(5)	171(4)[h]
O6-H62 ··· N2	0.84(5)	1.94(5)	2.704(5)	151(4)
O7-H71 ··· O20	0.84(5)	1.95(5)	2.820(5)	173(5)[h]
O7-H72 ··· N10	0.84(4)	2.06(4)	2.892(5)	172(4)[f]
O8-H81 ··· O17	0.85(4)	1.89(3)	2.735(5)	174(5)[h]
O8-H82 ··· N11	0.87(5)	2.10(5)	2.944(6)	165(6)[c]
O11-H111··· N4	0.87(5)	1.88(5)	2.710(5)	176(4)
O11-H112 ··· O15	0.83(4)	1.93(4)	2.748(5)	167(5)[h]
O12-H121 ··· O19	0.83(5)	1.90(5)	2.723(5)	173(7)
O12-H122 ··· O11	0.85(4)	1.84(4)	2.676(4)	171(6)
O13-H131 ··· N6	0.89(5)	2.04(6)	2.921(10)	173(5)
O13-H132 ··· O18	0.84(5)	2.15(6)	2.927(10)	153(5)[i]
O13-H132 ··· O22A	0.84(5)	2.32(6)	2.841(10)	121(5)[i]
O14-H141 ··· O12	0.79(5)	2.10(5)	2.861(5)	160(4)[j]
O14-H142 ··· N13	0.83(5)	1.91(5)	2.730(5)	175(4)[a]
O15-H151 ··· N12	0.83(5)	1.93(5)	2.741(5)	168(5)[b]
O15-H152 ··· O14	0.84(5)	1.96(5)	2.776(5)	166(5)[c]

O16-H161 ··· O17	0.87(5)	1.88(4)	2.742(5)	168(6)
O16-H162 ··· N7	0.84(5)	2.11(4)	2.8917(5)	154(6)[i]
O17-H171 ··· O19	0.83(5)	2.01(5)	2.801(5)	158(5)
O17-H172 ··· N16	0.85(6)	1.95(6)	2.789(5)	168(4)[a]
O18-H181 ··· N15	0.87(5)	1.95(5)	2.814(5)	166(6)[a]
O19-H191 ··· O15	0.87(5)	1.87(5)	2.729(5)	173(5)
O19-H192 ··· O21	0.85(5)	1.90(6)	2.738(5)	169(6)
O20-H201 ··· O18	0.86(3)	1.87(4)	2.709(6)	165(4)[i]
O21-H212 ··· O13	0.85(6)	2.38(6)	3.060(5)	138(6)
O21-H212 ··· O22B	0.85(5)	2.30(6)	2.787(5)	117(5)[k]

Symmetry opeartion

[a] = 1/2+x,1/2-y,1/2+z
[b] = x,y,1+z
[c] = -1/2+x,1/2-y,1/2+z
[d] = 1/2-x,1/2+y,3/2-z
[e] = 1-x,1-y,1-z
[f] = 1/2-x,1/2+y,1/2-z
[g] = 3/2-x,1/2+y,3/2-z
[h] = -1/2+x,1/2-y,-1/2+z
[k] = -1+x,y,z
[i] = 1-x,-y,1-z
[j] = 1+x,y,z

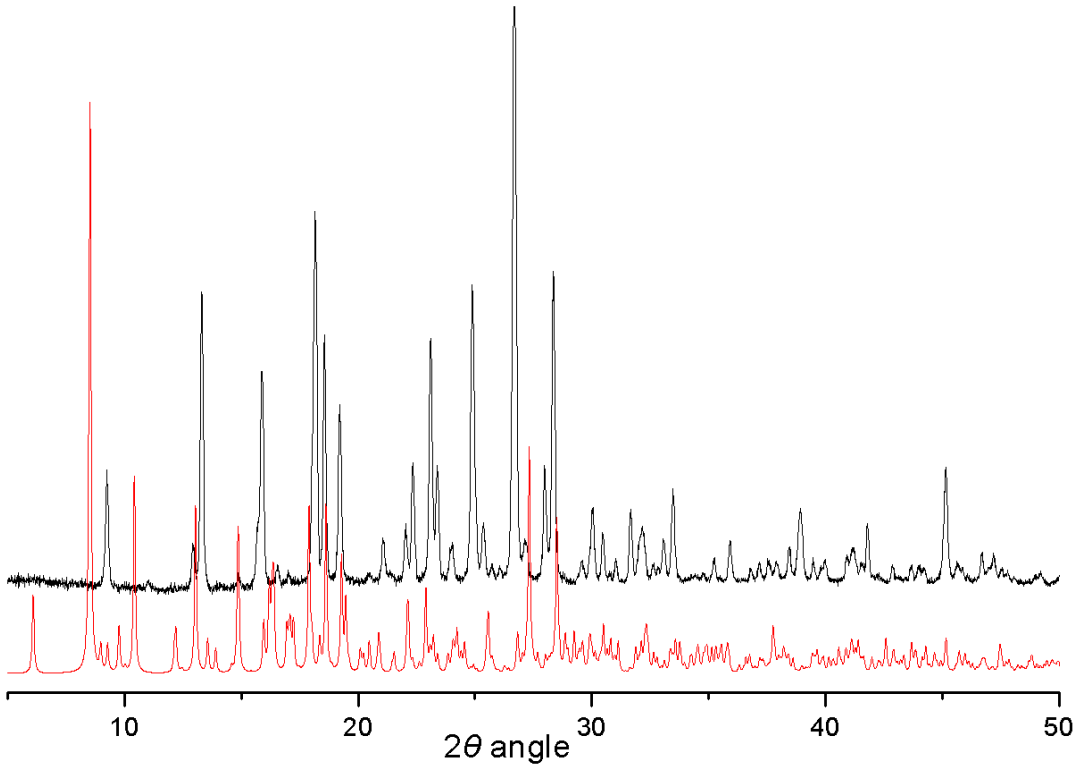

Fig. S2 X-ray powder pattern for the product formed hydrothermally (black) with the calculated pattern (red) for **1** for comparison.