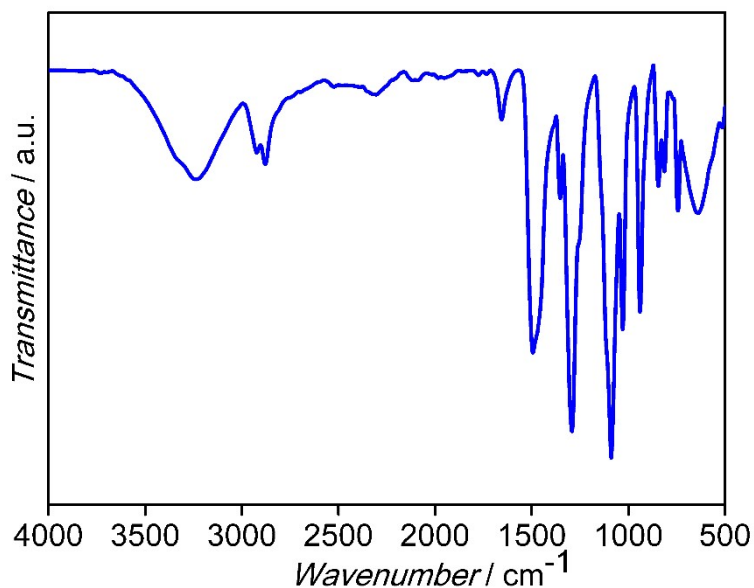
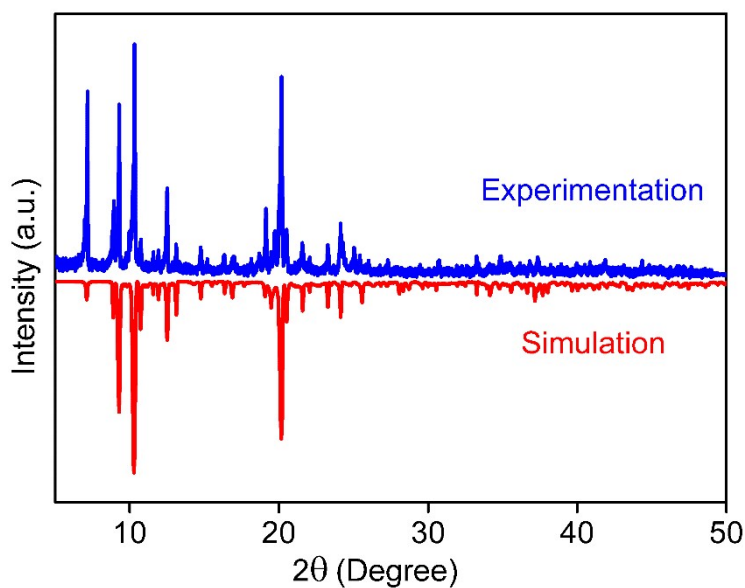


### Supporting Information



**Figure S1.** IR spectrum of **1** measured at room temperature.



**Figure S2.** PXRD pattern **1** measured at room temperature.

**Table S1.** Hydrogen bonds for **1** at 173 K [Å and deg].

D-H···A	D-H	H···A	D···A	D···H-A
C(12 <sup>a</sup> )-H(12A <sup>a</sup> )···O(19) #1	0.99	2.53	3.50(2)	165.6
C(14)-H(14B)···O(17)	0.99	2.58	3.547(15)	129.8
C(16)-H(16A)···O(19) #2	0.99	2.56	3.547(15)	176.0

C(19)–H(19B)···O(13) #3	0.99	2.50	3.294(19)	137.5
O(20)–H(20C)···O(5 <sup>a</sup> )	0.90	1.93	2.61(2)	130.7
O(20)–H(20C)···O(5A <sup>b</sup> )	0.90	2.30	2.93(2)	126.9
O(20)–H(20D)···O(3 <sup>a</sup> )	0.90	2.14	2.73(3)	122.9
O(20)–H(20D)···O(4 <sup>a</sup> )	0.90	2.16	3.01(3)	157.2
O(20)–H(20D)···O(3A <sup>b</sup> )	0.90	2.58	3.270(18)	134.3
O(20)–H(20D)···O(4A <sup>b</sup> )	0.90	2.23	3.00(2)	143.4
O(21)–H(21A)···O(11) #4	0.90	2.12	2.701(15)	121.5
O(21)–H(21B)···O(2 <sup>a</sup> )	1.00	2.15	3.11(2)	162.5
O(21)–H(21B)···O(2A <sup>b</sup> )	1.00	1.84	2.818(17)	166.5
O(22)–H(22A)···O(9)	0.88	1.93	2.755(15)	155.0
O(22)–H(22B)···O(7)	0.96	2.03	2.792(13)	135.3
O(24)–H(24A)···O(4 <sup>a</sup> )	0.90	2.08	2.95(3)	1627
O(24)–H(24A)···O(4A <sup>b</sup> )	0.90	1.90	2.786(18)	168.2
O(24)–H(24B)···O(12)	0.90	2.32	2.809(13)	114.4
O(24)–H(24B)···O(13)	0.90	2.64	3.353(15)	137.0

Symmetry codes: #1  $-x+1, -y+1, -z+1$ ; #2  $-x+1, -y+2, -z+1$ ; #3  $-x+2, -y+1, -z+1$ ; #4  $x, y+1, z$ .

**Table S2.** Torsion angles [ $^{\circ}$ ] for 15-crown-5 of **1** at 173 K and 293 K.

173 K		293 K	
O(5)–C(1)–C(2)–O(1)	–49(3)	C(11)–C(12)–O(6)–C(13)	–161(9)
O(1)–C(3)–C(4)–O(2)	–18(4)	C(12)–C(11)–O(10)–C(20)	127(9)
O(2)–C(5)–C(6)–O(3)	20(4)	C(13)–C(14)–O(7)–C(15)	–147(6)
O(3)–C(7)–C(8)–O(4)	–22(4)	C(14)–C(13)–O(6)–C(12)	–169(6)
O(4)–C(9)–C(10)–O(5)	–21(4)	C(15)–C(16)–O(8)–C(17)	–152(5)
O(6)–C(11)–C(12)–O(10)	–64(2)	C(16)–C(15)–O(7)–C(14)	158(7)
O(10)–C(13)–C(14)–O(9)	66.1(17)	C(17)–C(18)–O(9)–C(19)	154(7)
O(9)–C(15)–C(16)–O(8)	70.1(16)	C(18)–C(17)–O(8)–C(16)	150(6)
O(8)–C(17)–C(18)–O(7)	–69.9(16)	C(19)–C(20)–O(10)–C(11)	–137(9)
O(7)–C(19)–C(20)–O(6)	–76.8(17)	C(20)–C(19)–O(9)–C(18)	–149(6)
O(5A)–C(1A)–C(2A)–O(1A)	71(3)	O(6)–C(13)–C(14)–O(7)	–32(7)
O(1A)–C(3A)–C(4A)–O(2A)	–44(3)	O(7)–C(15)–C(16)–O(8)	–22(8)
O(2A)–C(5A)–C(6A)–O(3A)	80(3)	O(8)–C(17)–C(18)–O(9)	24(5)
O(3A)–C(7A)–C(8A)–O(4A)	–80(3)	O(9)–C(19)–C(20)–O(10)	–21(8)
O(4A)–C(9A)–C(10A)–O(5A)	–65(3)	O(9)–C(18A)–C(17A)–O(8A)	–71.1(19)
C(4)–C(3)–O(1)–C(2)	–132(3)	O(10)–C(11)–C(12)–O(6)	32(6)
C(1)–C(2)–O(1)–C(3)	–176(2)	O(14)–N(3)–O(15)–Y(1)	4.7(15)
C(6)–C(5)–O(2)–C(4)	–140(2)	O(15)–N(3)–O(14)–Y(1)	–4.9(16)
C(3)–C(4)–O(2)–C(5)	145(2)	O(16)–N(3)–O(14)–Y(1)	–179.5(13)
C(5)–C(6)–O(3)–C(7)	156(2)	O(16)–N(3)–O(15)–Y(1)	179.4(13)
C(8)–C(7)–O(3)–C(6)	–159(3)	O(17)–N(2)–O(19)–Y(1)	–6.9(17)
C(10)–C(9)–O(4)–C(8)	–118(3)	O(18)–N(2)–O(17)–Y(1)	–178.8(17)

C(7)–C(8)–O(4)–C(9)	152(3)	O(18)–N(2)–O(19)–Y(1)	179(2)
C(2)–C(1)–O(5)–C(10)	–116(3)	O(19)–N(2)–O(17)–Y(1)	6.6(16)
C(9)–C(10)–O(5)–C(1)	166(2)	C(1)–C(2)–O(1)–C(3)	–165(2)
C(1A)–C(2A)–O(1A)–C(3A)	150(3)	C(2)–C(1)–O(5)–C(10)	–124(3)
C(4A)–C(3A)–O(1A)–C(2A)	–140(3)	C(3)–C(4)–O(2)–C(5)	123(4)
C(6A)–C(5A)–O(2A)–C(4A)	–162(2)	C(4)–C(3)–O(1)–C(2)	–141(3)
C(3A)–C(4A)–O(2A)–C(5A)	133(2)	C(5)–C(6)–O(3)–C(7)	–174(3)
C(5A)–C(6A)–O(3A)–C(7A)	–171.9(19)	C(6)–C(5)–O(2)–C(4)	–152(3)
C(8A)–C(7A)–O(3A)–C(6A)	180(2)	C(7)–C(8)–O(4)–C(9)	147(2)
C(10A)–C(9A)–O(4A)–C(8A)	–72(3)	C(8)–C(7)–O(3)–C(6)	179(3)
C(7A)–C(8A)–O(4A)–C(9A)	156(2)	C(9)–C(10)–O(5)–C(1)	167(3)
C(2A)–C(1A)–O(5A)–C(10A)	–169(2)	C(10)–C(9)–O(4)–C(8)	–123(3)
C(9A)–C(10A)–O(5A)–C(1A)	155(2)	O(1)–C(3)–C(4)–O(2)	7(5)
		O(2)–C(5)–C(6)–O(3)	37(4)
		O(3)–C(7)–C(8)–O(4)	–38(4)
		O(4)–C(9)–C(10)–O(5)	–19(4)
		O(5)–C(1)–C(2)–O(1)	–48(3)
		C(1A)–C(2A)–O(1A)–C(3A)	176(4)
		C(2A)–C(1A)–O(5A)–C(10A)	172(4)
		C(3A)–C(4A)–O(2A)–C(5A)	152(4)
		C(4A)–C(3A)–O(1A)–C(2A)	–105(7)
		C(5A)–C(6A)–O(3A)–C(7A)	176(4)
		C(6A)–C(5A)–O(2A)–C(4A)	–92(5)
		C(7A)–C(8A)–O(4A)–C(9A)	53(5)
		C(8A)–C(7A)–O(3A)–C(6A)	–152(4)
		C(9A)–C(10A)–O(5A)–C(1A)	–163(4)
		C(10A)–C(9A)–O(4A)–C(8A)	–152(4)
		O(1A)–C(3A)–C(4A)–O(2A)	–46(7)
		O(2A)–C(5A)–C(6A)–O(3A)	–94(5)
		O(3A)–C(7A)–C(8A)–O(4A)	90(5)
		O(4A)–C(9A)–C(10A)–O(5A)	87(6)
		O(5A)–C(1A)–C(2A)–O(1A)	–78(7)
		C(11A)–C(12A)–O(6A)–C(13A)	–164.2(17)
		C(11A)–O(10A)–C(20A)–C(19A)	–164.4(15)
		C(12A)–C(11A)–O(10A)–C(20A)	84(2)
		C(12A)–O(6A)–C(13A)–C(14A)	168(2)
		O(10A)–C(11A)–C(12A)–O(6A)	71(2)
		O(10A)–C(20A)–C(19A)–O(9)	68(2)
		O(6A)–C(13A)–C(14A)–O(7A)	–55(3)
		C(13A)–C(14A)–O(7A)–C(15A)	–96(2)
		C(19A)–O(9)–C(18A)–C(17A)	171.3(13)
		C(14A)–O(7A)–C(15A)–C(16A)	–178.6(17)
		O(7A)–C(15A)–C(16A)–O(8A)	–78(2)
		C(18A)–O(9)–C(19A)–C(20A)	–169.4(13)

C(18A)–C(17A)–O(8A)–C(16A)	170.6(14)
C(15A)–C(16A)–O(8A)–C(17A)	–83(2)

**Table S3.** Selected bond lengths [Å] and angles [°] for **1** (173 K, 293 K).

<b>1</b> –173 K			
Y1–O14	2.416 (11)	O23–Y1–O22	73.5 (3)
Y1–O16	2.442 (10)	O20–Y1–O21	76.0 (3)
Y1–O17	2.436 (10)	O22–Y1–O21	78.3 (3)
Y1–O18	2.506 (10)	O23–Y1–O24	69.3 (3)
Y1–O20	2.337 (8)	O20–Y1–O24	71.5 (3)
Y1–O21	2.366 (8)	O23–Y1–O14	75.8 (4)
Y1–O22	2.357 (8)	O20–Y1–O14	80.4 (4)
Y1–O23	2.325 (8)	O22–Y1–O14	94.5 (4)
Y1–O24	2.372 (8)	O24–Y1–O14	78.7 (4)
		O23–Y1–O17	75.0 (3)
		O22–Y1–O17	71.8 (3)
		O21–Y1–O17	78.9 (3)
		O24–Y1–O17	96.3 (4)
		O20–Y1–O16	76.6 (4)
		O22–Y1–O16	72.8 (4)
		O21–Y1–O16	75.2 (3)
		O14–Y1–O16	51.2 (3)
		O20–Y1–O18	75.4 (4)
		O21–Y1–O18	69.8 (4)
		O24–Y1–O18	72.9 (4)
		O17–Y1–O18	51.2 (3)
<b>1</b> –293 K			
Y1–O14	2.453 (12)	O(14)–Y(1)–O(15)	50.4(4)
Y1–O15	2.547 (13)	O(17)–Y(1)–O(14)	140.9(4)
Y1–O17	2.419 (12)	O(17)–Y(1)–O(15)	140.1(4)
Y1–O19	2.367 (13)	O(19)–Y(1)–O(14)	148.8(5)
Y1–O20	2.350 (9)	O(19)–Y(1)–O(15)	147.4(5)
Y1–O21	2.369 (10)	O(19)–Y(1)–O(17)	51.7(4)
Y1–O22	2.321 (10)	O(19)–Y(1)–O(21)	127.4(4)
Y1–O23	2.411 (11)	O(19)–Y(1)–O(23)	76.8(5)
Y1–O24	2.338 (10)	O(20)–Y(1)–O(14)	72.2(4)
		O(20)–Y(1)–O(15)	117.6(4)
		O(20)–Y(1)–O(17)	73.4(4)
		O(20)–Y(1)–O(19)	94.4(5)
		O(20)–Y(1)–O(21)	77.6(4)
		O(20)–Y(1)–O(23)	142.8(4)
		O(21)–Y(1)–O(14)	78.3(4)

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O(21)-Y(1)-O(15)	69.6(4)
O(21)-Y(1)-O(17)	76.6(4)
O(21)-Y(1)-O(23)	136.2(4)
O(22)-Y(1)-O(14)	123.3(5)
O(22)-Y(1)-O(15)	73.2(5)
O(22)-Y(1)-O(17)	78.8(4)
O(22)-Y(1)-O(19)	83.8(5)
O(22)-Y(1)-O(20)	145.5(4)
O(22)-Y(1)-O(21)	76.4(4)
O(22)-Y(1)-O(23)	70.4(4)
O(22)-Y(1)-O(24)	137.7(4)
O(23)-Y(1)-O(14)	96.7(4)
O(23)-Y(1)-O(15)	74.0(5)
O(23)-Y(1)-O(17)	122.1(4)
O(24)-Y(1)-O(14)	73.3(4)
O(24)-Y(1)-O(15)	106.0(4)
O(24)-Y(1)-O(17)	113.8(5)
O(24)-Y(1)-O(19)	75.9(5)
O(24)-Y(1)-O(20)	73.8(4)
O(24)-Y(1)-O(21)	144.5(4)
O(24)-Y(1)-O(23)	69.0(4)

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