Electronic Supplementary Material for CrystEngComm

Supplementary information

Hydrogen Bonding in the Perhydrate and Hydrates of 1,4-Diazabicyclo[2.2.2]octane (DABCO)

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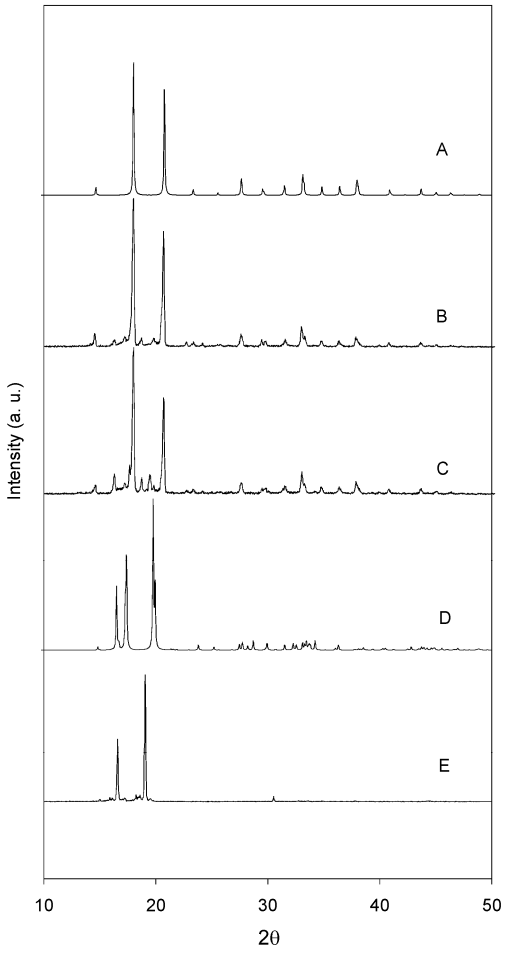

Fig. S1 The calculated XRPD pattern of DABCO bis(perhydrate) **1** (A) and observed (at 173 K) patterns of bulk **1** crystallized at +5°C (B), at –5°C (C), the monohydrate **2** (D), and sublimed DABCO (E).

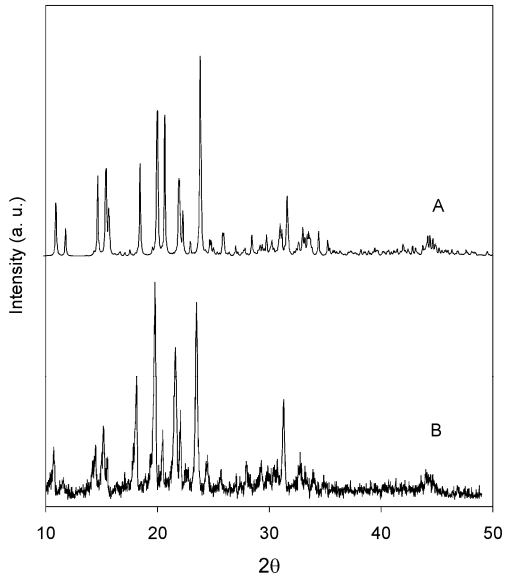

Fig. S2 The calculated (A) and observed (B) XRPD pattern of DABCO hexahydrate **3** at 173 K.

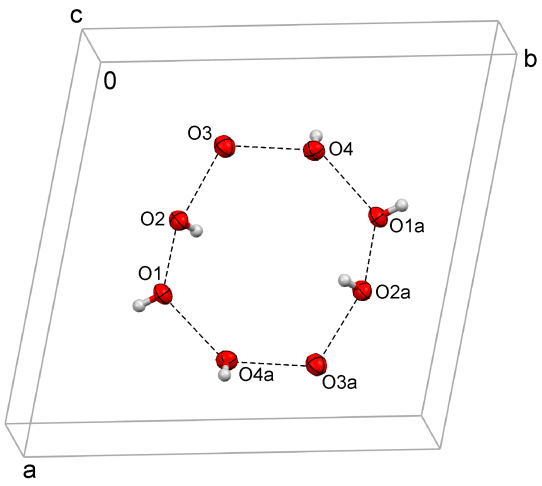

Fig. S3 Water ring A in **3**. Symmetry code: (a) 1–*x*, 1–*y*, –*z*.

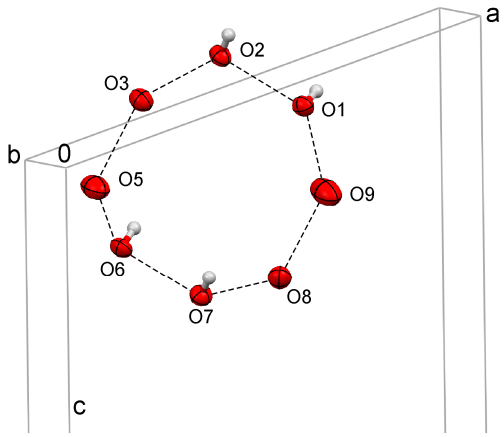

Fig. S4 Water ring B in **3**.

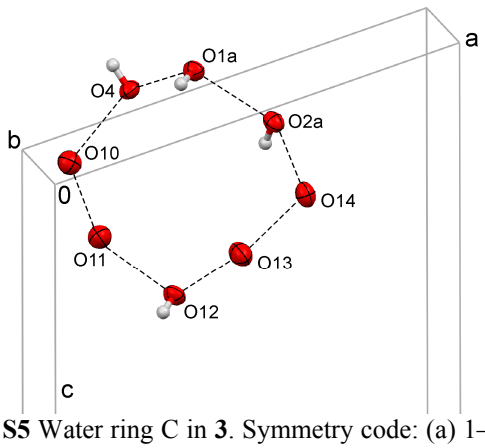

Fig. S5 Water ring C in **3**. Symmetry code: (a) 1–*x*, 1–*y*, –*z*.

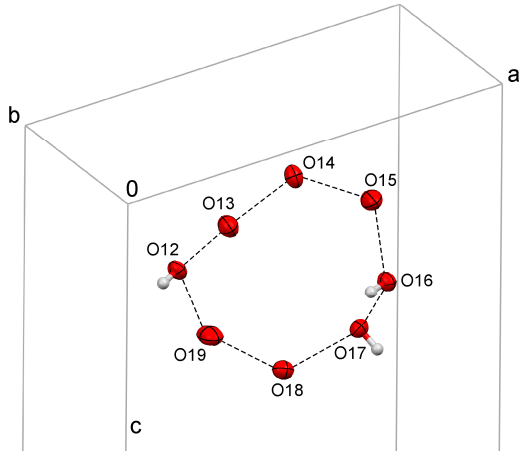

Fig. S6 Water ring D in **3**.

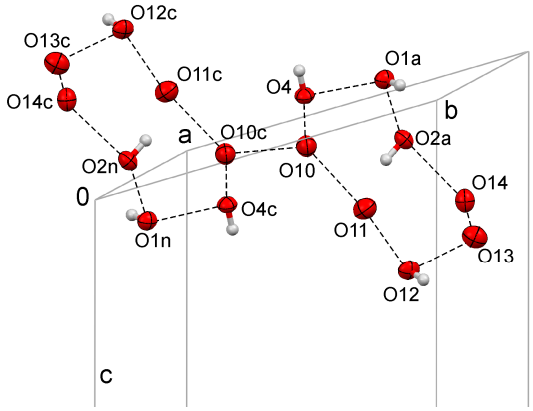

Fig. S7 Water rings C and Cc in **3** connected by inversion through the O10...O10c interaction. Symmetry code: (a) 1–*x*, 1–*y*, –*z*; (c) –*x*, 1–*y*, –*z*; (n) –1+*x*, *y*, *z*.

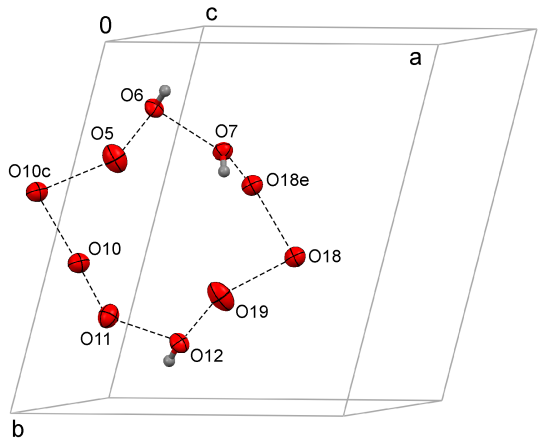

Fig. S8 Cyclic water decamer in **3** created by the O10...O10c and O18...O18e interactions. Symmetry code: (c) –*x*, 1–*y*, –*z*; (e) 1–*x*, 1–*y*, 1–*z*.

Table S1 Interatomic distances (Å) and angles (°) for the hexahydrate **3**

O(1)-N(1)	2.719(4)	O(14)-O(2)#1	2.788(12)
O(1)-O(9)	2.724(7)	O(14)-O(15)	2.829(10)
O(1)-O(2)	2.786(3)	O(15)-O(16)	2.713(6)
O(1)-O(4)#1	2.823(3)	O(15)-O(20)#1	2.822(7)
O(2)-N(2)	2.735(3)	O(16)-N(44)#8	2.710(4)
O(2)-O(3)	2.787(6)	O(16)-O(23)#9	2.783(4)
O(2)-O(14)#1	2.788(12)	O(16)-O(17)	2.815(3)
O(3)-O(4)	2.784(5)	O(17)-N(33)#10	2.723(3)
O(3)-O(20)	2.795(13)	O(17)-O(24)#3	2.796(6)
O(3)-O(5)	2.821(7)	O(17)-O(18)	2.804(11)
O(4)-N(3)	2.708(3)	O(18)-O(18)#5	2.77(2)
O(4)-O(10)	2.813(11)	O(18)-O(7)#5	2.779(11)
O(4)-O(1)#1	2.823(3)	O(18)-O(19)	2.815(10)
O(5)-O(6)	2.720(7)	O(19)-O(24)#11	2.819(6)
O(5)-O(10)#2	2.808(11)	O(20)-O(21)	2.774(6)
O(6)-N(11)#3	2.719(4)	O(20)-O(15)#1	2.822(7)
O(6)-O(21)#4	2.780(4)	O(20)-O(11)#2	2.824(7)
O(6)-O(7)	2.809(3)	O(21)-O(6)#4	2.780(4)
O(7)-N(22)#1	2.729(3)	O(21)-O(22)	2.823(12)
O(7)-O(18)#5	2.779(11)	O(22)-O(14)#1	2.73(2)
O(7)-O(8)	2.793(6)	O(22)-O(23)	2.751(12)
O(8)-O(24)#3	2.722(12)	O(22)-O(9)#3	2.788(12)
O(8)-O(9)	2.789(7)	O(23)-O(24)	2.740(6)
O(8)-O(13)#6	2.865(6)	O(23)-O(16)#12	2.783(4)
O(9)-O(22)#3	2.788(12)	O(24)-O(8)#3	2.722(12)
O(10)-O(11)	2.766(12)	O(24)-O(17)#3	2.796(6)
O(10)-O(10)#2	2.77(2)	O(24)-O(19)#13	2.819(6)
O(10)-O(5)#2	2.808(11)	N(11)-O(6)#3	2.719(4)
O(11)-O(12)	2.805(4)	N(22)-O(7)#1	2.729(3)
O(11)-O(20)#2	2.824(7)	N(33)-O(17)#14	2.723(3)
O(12)-O(19)	2.713(7)	N(44)-O(16)#8	2.710(4)
O(12)-N(4)	2.714(4)		
O(12)-O(13)	2.779(4)	N(1)-O(1)-O(9)	93.20(16)
O(13)-O(14)	2.754(11)	N(1)-O(1)-O(2)	103.48(11)
O(13)-O(8)#7	2.865(6)	O(9)-O(1)-O(2)	136.42(17)
O(14)-O(22)#1	2.73(2)	N(1)-O(1)-O(4)#1	102.31(11)
		O(9)-O(1)-O(4)#1	105.80(19)
		O(2)-O(1)-O(4)#1	109.35(11)
		N(2)-O(2)-O(1)	101.57(10)

N(2)-O(2)-O(3)	105.95(14)	O(1)-O(9)-O(8)	136.1(3)
O(1)-O(2)-O(3)	121.08(16)	O(22)#3-O(9)-O(8)	100.5(4)
N(2)-O(2)-O(14)#1	86.4(3)	O(11)-O(10)-O(10)#2	122.9(6)
O(1)-O(2)-O(14)#1	126.0(2)	O(11)-O(10)-O(5)#2	99.3(4)
O(3)-O(2)-O(14)#1	106.9(2)	O(10)#2-O(10)-O(5)#2	84.4(4)
O(4)-O(3)-O(2)	110.2(2)	O(11)-O(10)-O(4)	120.8(4)
O(4)-O(3)-O(20)	112.8(3)	O(10)#2-O(10)-O(4)	107.5(6)
O(2)-O(3)-O(20)	100.6(2)	O(5)#2-O(10)-O(4)	115.5(4)
O(4)-O(3)-O(5)	105.2(2)	O(10)-O(11)-O(12)	144.1(2)
O(2)-O(3)-O(5)	134.9(2)	O(10)-O(11)-O(20)#2	101.3(2)
O(20)-O(3)-O(5)	90.2(3)	O(12)-O(11)-O(20)#2	113.81(16)
N(3)-O(4)-O(3)	106.00(16)	O(19)-O(12)-N(4)	98.37(15)
N(3)-O(4)-O(10)	98.1(2)	O(19)-O(12)-O(13)	119.00(17)
O(3)-O(4)-O(10)	94.0(3)	N(4)-O(12)-O(13)	98.89(12)
N(3)-O(4)-O(1)#1	101.85(10)	O(19)-O(12)-O(11)	122.89(19)
O(3)-O(4)-O(1)#1	137.64(17)	N(4)-O(12)-O(11)	99.35(12)
O(10)-O(4)-O(1)#1	113.0(3)	O(13)-O(12)-O(11)	111.08(12)
O(6)-O(5)-O(10)#2	138.2(3)	O(14)-O(13)-O(12)	122.6(3)
O(6)-O(5)-O(3)	122.2(2)	O(14)-O(13)-O(8)#7	117.1(3)
O(10)#2-O(5)-O(3)	96.5(3)	O(12)-O(13)-O(8)#7	118.91(17)
N(11)#3-O(6)-O(5)	96.72(15)	O(22)#1-O(14)-O(13)	92.7(6)
N(11)#3-O(6)-O(21)#4	99.59(12)	O(22)#1-O(14)-O(2)#1	126.9(7)
O(5)-O(6)-O(21)#4	119.83(18)	O(13)-O(14)-O(2)#1	117.1(3)
N(11)#3-O(6)-O(7)	102.95(11)	O(22)#1-O(14)-O(15)	98.9(5)
O(5)-O(6)-O(7)	105.99(18)	O(13)-O(14)-O(15)	129.4(4)
O(21)#4-O(6)-O(7)	125.45(12)	O(2)#1-O(14)-O(15)	94.2(4)
N(22)#1-O(7)-O(18)#5	105.9(3)	O(16)-O(15)-O(20)#1	145.2(2)
N(22)#1-O(7)-O(8)	97.34(15)	O(16)-O(15)-O(14)	119.9(3)
O(18)#5-O(7)-O(8)	96.9(2)	O(20)#1-O(15)-O(14)	94.4(3)
N(22)#1-O(7)-O(6)	101.05(10)	N(44)#8-O(16)-O(15)	99.03(15)
O(18)#5-O(7)-O(6)	138.2(2)	N(44)#8-O(16)-O(23)#9	98.93(12)
O(8)-O(7)-O(6)	110.81(15)	O(15)-O(16)-O(23)#9	116.94(16)
O(24)#3-O(8)-O(9)	94.3(3)	N(44)#8-O(16)-O(17)	99.16(11)
O(24)#3-O(8)-O(7)	106.1(2)	O(15)-O(16)-O(17)	129.07(18)
O(9)-O(8)-O(7)	117.1(3)	O(23)#9-O(16)-O(17)	106.52(11)
O(24)#3-O(8)-O(13)#6	109.3(3)	N(33)#10-O(17)-O(24)#3	84.41(15)
O(9)-O(8)-O(13)#6	90.2(2)	N(33)#10-O(17)-O(18)	104.1(2)
O(7)-O(8)-O(13)#6	132.9(2)	O(24)#3-O(17)-O(18)	97.8(3)
O(1)-O(9)-O(22)#3	121.8(3)	N(33)#10-O(17)-O(16)	101.67(10)

O(24)#3-O(17)-O(16)	146.38(14)
O(18)-O(17)-O(16)	112.3(3)
O(18)#5-O(18)-O(7)#5	113.1(6)
O(18)#5-O(18)-O(17)	108.5(6)
O(7)#5-O(18)-O(17)	110.9(3)
O(18)#5-O(18)-O(19)	88.6(4)
O(7)#5-O(18)-O(19)	106.5(4)
O(17)-O(18)-O(19)	127.4(4)
O(12)-O(19)-O(18)	145.2(3)
O(12)-O(19)-O(24)#11	120.0(2)
O(18)-O(19)-O(24)#11	94.0(3)
O(21)-O(20)-O(3)	115.4(3)
O(21)-O(20)-O(15)#1	96.2(2)
O(3)-O(20)-O(15)#1	92.8(3)
O(21)-O(20)-O(11)#2	118.8(2)
O(3)-O(20)-O(11)#2	106.1(2)
O(15)#1-O(20)-O(11)#2	125.2(3)
O(20)-O(21)-O(6)#4	121.76(18)
O(20)-O(21)-O(22)	112.2(3)
O(6)#4-O(21)-O(22)	122.4(3)
O(14)#1-O(22)-O(23)	111.5(6)
O(14)#1-O(22)-O(9)#3	99.7(5)
O(23)-O(22)-O(9)#3	95.1(4)
O(14)#1-O(22)-O(21)	92.9(6)
O(23)-O(22)-O(21)	127.4(4)
O(9)#3-O(22)-O(21)	126.8(5)
O(24)-O(23)-O(22)	111.0(3)
O(24)-O(23)-O(16)#12	123.48(18)
O(22)-O(23)-O(16)#12	123.0(3)
O(8)#3-O(24)-O(23)	98.8(2)
O(8)#3-O(24)-O(17)#3	122.9(3)
O(23)-O(24)-O(17)#3	114.9(2)
O(8)#3-O(24)-O(19)#13	91.3(3)
O(23)-O(24)-O(19)#13	129.5(3)
O(17)#3-O(24)-O(19)#13	99.6(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x,-y+1,-z #3 -x+1,-y,-z
#4 -x,-y,-z #5 -x+1,-y+1,-z+1 #6 x,y-1,z
#7 x,y+1,z #8 -x+1,-y+2,-z+1 #9 x+1,y+1,z+1
#10 x+1,y,z+1 #11 x,y+1,z+1 #12 x-1,y-1,z-1
#13 x,y-1,z-1 #14 x-1,y,z-1

The atom numbering is in accordance with the CIF file CCDC 634614.