Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Sample preparation

Aqueous solution (30 mL) containing Dabco (0.56 g, 5 mmol), $NaBF_4$ (0.55 g, 5 mmol) and HBF_4 (3.07 g, 35 mmol) was evaporated to afford colourless block crystals of **1**.

1: yield 80% (based on $NaBF_4$). Elemental analysis calcd (%) for $C_{12}H_{28}B_6F_{24}N_4Na_2$ (795.22): C 18.13, H 3.55, N 7.05; found: C 18.22, H 3.50, N 7.04.

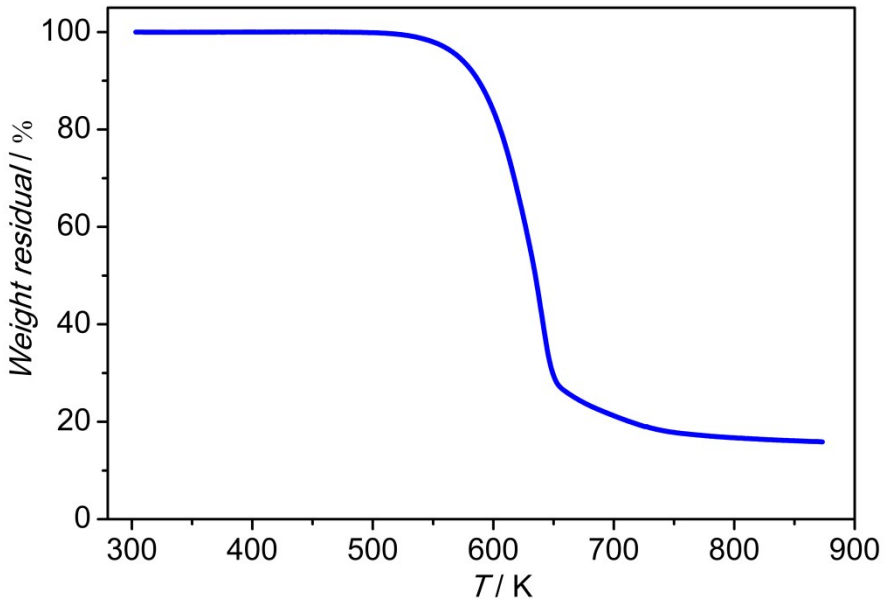

Figure S1. TGA curves of **1**.

Table S1. Bond lengths (Å) and bond angles (°) for **1**.

293 K			
Na1−F1	2.847(3)	Na1−F1−B1	107.1(2)
Na1−F1#3	2.847(3)	Na2−F4−B1	126.9(2)
Na1−F1#4	2.847(3)	F1−Na1−F1#3	114.20(6)
Na1−F1#5	2.847(3)	F1−Na1−F1#4	65.80(6)
Na1−F1#6	2.847(3)	F1−Na1−F1#5	180.0
Na1−F1#7	2.847(3)	F1−Na1−F1#6	65.80(6)
Na2−F4	2.496(3)	F1−Na1−F1#7	114.20(6)
Na2−F4#1	2.496(3)	F1#3−Na1−F1#4	180.0
Na2−F4#2	2.496(3)	F1#3−Na1−F1#5	65.80(6)
Na2−F4#8	2.496(3)	F1#3−Na1−F1#6	114.20(6)

Na2−F4#9	2.496(3)	F1#3−Na1−F1#7	65.80(6)
Na2−F4#10	2.496(3)	F1#4−Na1−F1#5	114.20(6)
		F1#4−Na1−F1#6	65.80(6)
		F1#4−Na1−F1#7	114.20(6)
		F1#5−Na1−F1#6	114.20(6)
		F1#5−Na1−F1#7	65.80(6)
		F1#6−Na1−F1#7	180.0
		F4−Na2−F4#1	105.19(6)
		F4−Na2−F4#2	105.19(6)
		F4−Na2−F4#8	180.0
		F4−Na2−F4#9	74.81(6)
		F4−Na2−F4#10	74.81(6)
		F4#1−Na2−F4#2	105.19(6)
		F4#1−Na2−F4#8	74.81(6)
		F4#1−Na2−F4#9	74.81(6)
		F4#1−Na2−F4#10	180.0
		F4#2−Na2−F4#8	74.81(6)
		F4#2−Na2−F4#9	180.0
		F4#2−Na2−F4#10	74.81(6)
		F4#8−Na2−F4#9	105.19(6)
		F4#8−Na2−F4#10	105.19(6)
		F4#9−Na2−F4#10	105.19(6)

Symmetry codes: #1 z, x, y; #2 y, z, x; #3 −y+1/2, z−1/2, x; #4 y+1/2, −z+1/2, −x+1; #5 −x+1, −y, −z+1; #6 −z+1, x−1/2, −y+1/2; #7 z, −x+1/2, y+1/2; #8 −x+1, −y+1, −z+1; #9 −y+1, −z+1, −x+1; #10 −z+1, −x+1, −y+1.

Table S2. Hydrogen bonds (Å, °) for **1** at 293 K.

D−H···A	D−H	D···A	D−H···A
N1−H1C···F2	0.98	2.896(3)	124
N1−H1C···F2 [z, x, y]	0.98	2.896(3)	124
N1−H1C···F2 [y, z, x]	0.98	2.896(3)	124
N2−H2C···F1 [x−1/2, y, −z+1/2]	0.98	2.931(3)	127
N2−H2C···F1 [−z+1/2, x−1/2, y]	0.98	2.931(3)	127
N2−H2C···F1 [y, −z+1/2, x−1/2]	0.98	2.931(3)	127