Electronic Supplementary Information for Dalton Transactions

Supplementary Materials for

AlF·1,4-benzenedicarboxylate

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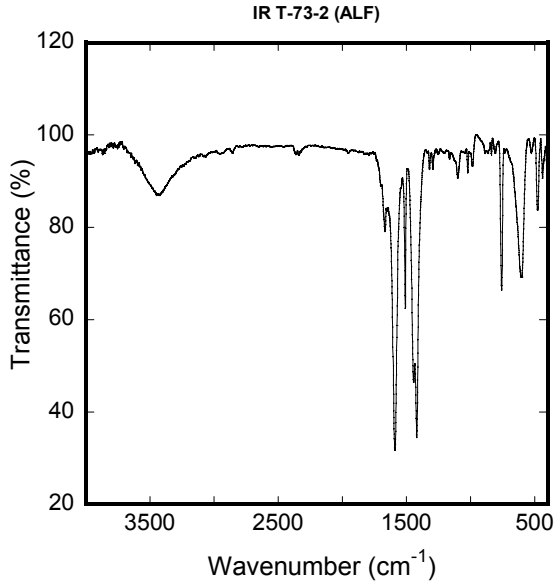

Figure S1. Infrared spectrum of ALF

Details of the X-ray refinement

The structure of AlF·1,4-benzenedicarboxylate was refined from laboratory X-ray data obtained using a Philips X'Pert Pro diffractometer and copper Kα radiation. The data were refined using GSAS with starting positions taken from the structure of Al(OH)BDC (MIL47ht).

Table S1 Crystallographic Data

chemical formula	AlFBDC
cryst syst	Orthorhombic
space group	*Imma*
a, Å	6.5502(7)
b, Å	16.250(4)
c, Å	13.378(2)
V, Å^3	1424.1(2)
Z	4
temp, K	293(2)
number of	360

reflections	
wRp	0.069
Rp	0.054

Table S2 Atom Positions for AlFBDC

	x	y	z
Al	0.25	0.25	0.75
F	0	0.25	0.692(1)
O	0.177(1)	0.1668(5)	0.8324(7)
C(1)	-0.193(1)	0.036(1)8	0.972(2)
C(2)	0	0.059(2)	0.959(2)
C(3)	0	0.129(1)	0.881(2)

The thermal parameters were fixed at values of 0.05.

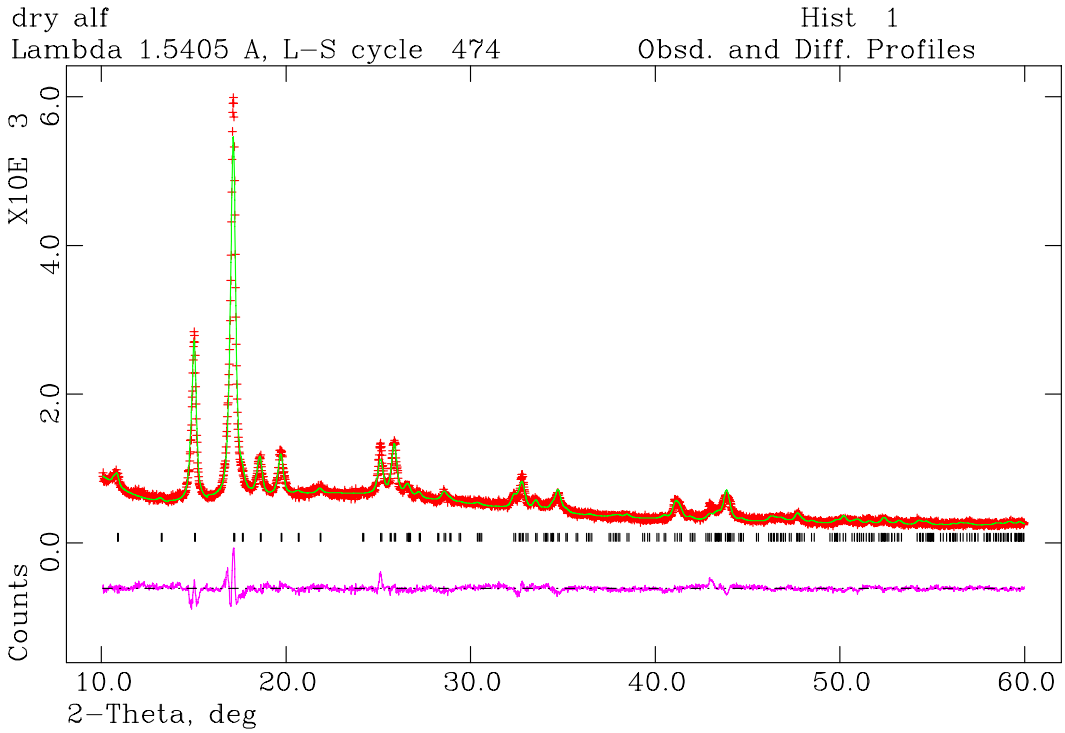

Figure S2. Observed (+) and calculated (-) powder diffraction data for ALF. The lower line is the difference between the observed data and calculated from the structure model. The vertical black lines mark the positions of the Bragg reflections.

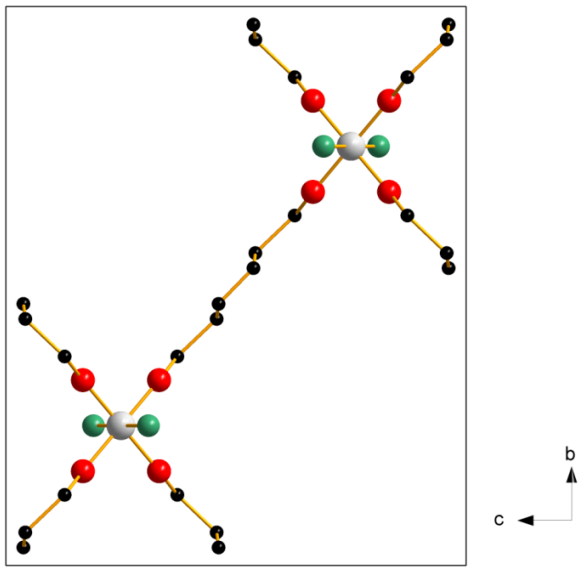

Figure S3. The structure of AlFBDC; the grey, green, red and black spheres represent aluminum, fluorine, oxygen and carbon atoms respectively.

Thermogravimetric sorption studies

The absorption of guest molecules by ALF was studied using a thermogravimetric procedure using the apparatus shown schematically in Figures S 4. A sample of ALF was first heated to 200 °C methane-helium gas flow in order to remove any molecules in the channels and the cooled to 28 °C. At constant weight, the methane-helium gas flow was switched to flow through a reservoir of the liquid guest molecules. This was achieved using a cross-over valve in order to maintain equal flow rates in the two gas streams. The behavior of thiophene is shown as a typical example in the text (Figure 5). As can be seen the introduction of thiophene at its saturated vapor pressure at ambient temperature produces a gain in weight which reaches a saturation value after ~ 60 min. The initial weight is recovered slowly by switching the gas stream back to pure methane-helium and rapidly when the temperature is raised to 150 °C.

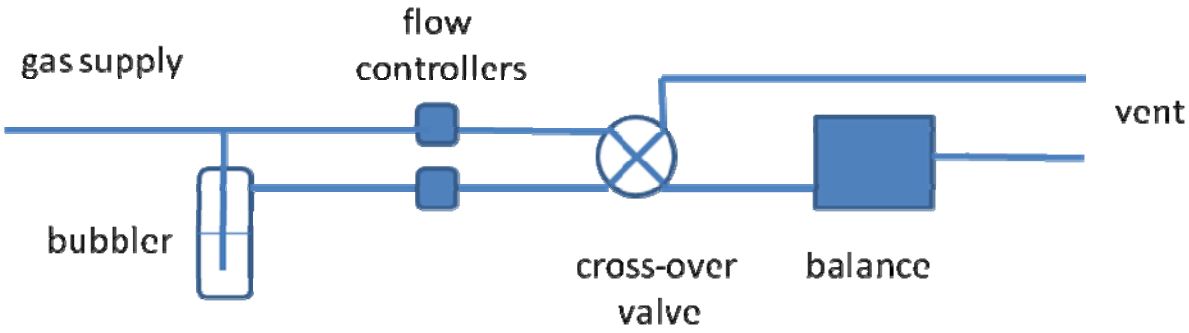

Figure S 4 A schematic diagram of the apparatus used thermogravimetric sorption studies.