Electronic Supplementary Material (ESI) for CrystEngComm

Hydrothermal synthesis, ab-initio structure determination and NMR study of the first mixed Cu/Al fluorinated MOF.

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Table S1 : Atomic positions and selected bond distance

Atom	x	y	z	Beq
Cu	0	0	0	1.47(6)
Al	¾	0.0646(7)	0.0182(2)	3.0(2)
Fa	¾	0.0691(1)	0.8022(2)	1.83(1)
Fb	0.6393(2)	0.0634(6)	0.9814(1)	1.83(1)
Fd	¾	0.8639(7)	0.0232(2)	1.83(1)
Fc	¾	0.0806(1)	0.2352(2)	1.83(1)
O	¾	0.2851(1)	0.0250(2)	1.83(1)
C1	0.10205	0.23140	0.15310	4.0(2)
C2	-0.01221	0.22358	0.28127	4.0(2)
N3	0.10362	0.34133	0.25426	4.0(2)
N4	0.03049	0.33755	0.33885	4.0(2)
N5	0.03114	0.15419	0.16461	4.0(2)
N6	-0.08859	0.18580	0.32656	4.0(2)
H7	-0.11366	0.23768	0.39875	8.10(1)
H8	-0.11235	0.10984	0.28330	8.10(1)
H9	0.14269	0.40480	0.26689	8.10(1)
H10	0.14417	0.20848	0.08177	8.10(1)

Cu-N4	2.0345	Al-FB	1.8339(2)
Cu-N5	2.0046	Al-FD	1.7927(2)
Cu-FB	2.3488(2)	Al-FC	1.8042(2)
Al-FA	1.7912(2)	Al-O	1.9709(2)

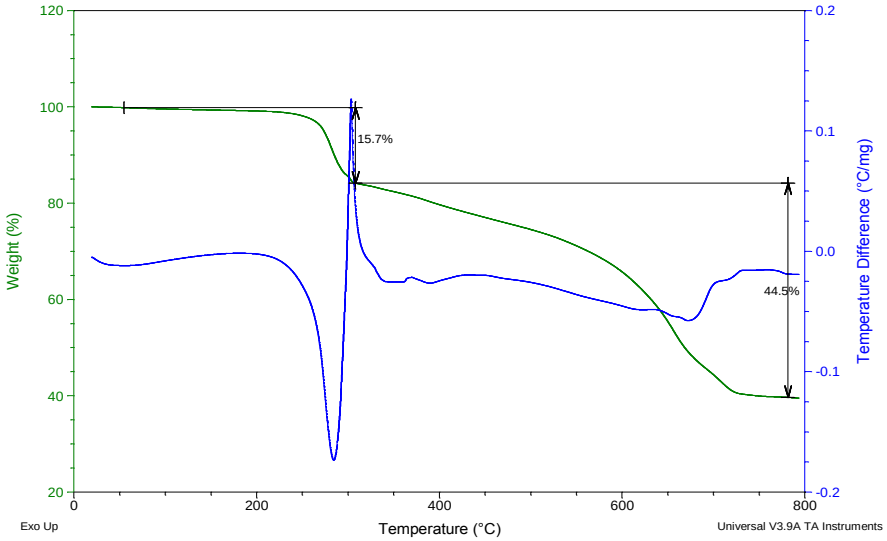

Fig. S1. Thermal analysis of $CuAlF_5(H_2O)[HAmTAZ]_2$ under argon.

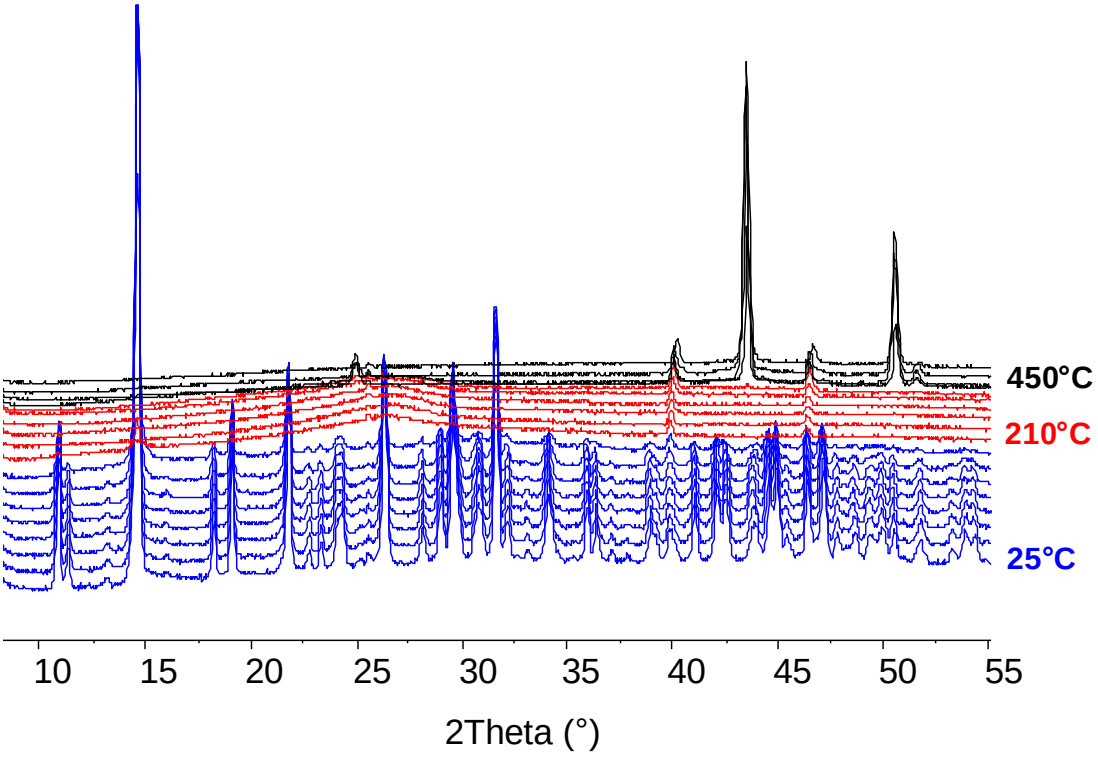

Fig. S2. Thermodiffraction of $CuAlF_5(H_2O)[HAmTAZ]_2$ under nitrogen.

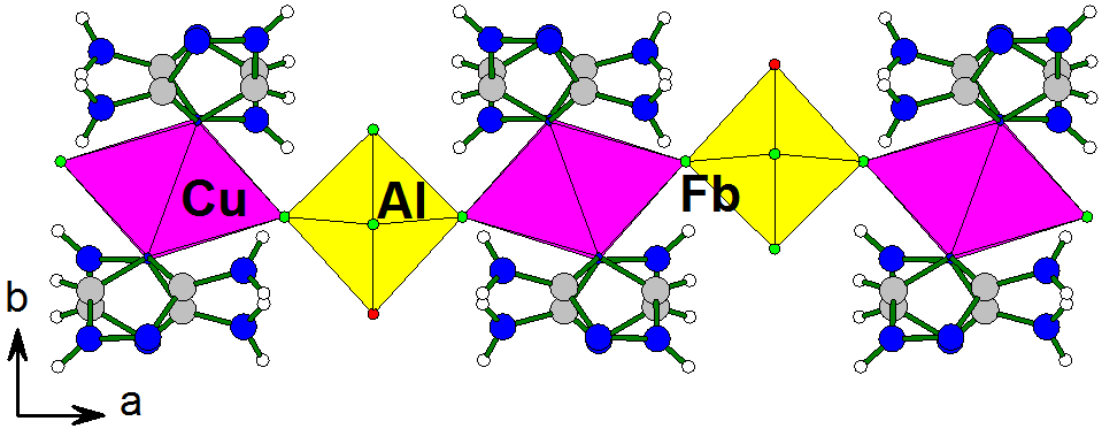

Fig. S3. CuN_4F_2 and AlF_5H_2O distorted octahedra *trans*-connected leading to inorganic chains along the *a* axis. Hydrogens are omitted for clarity.

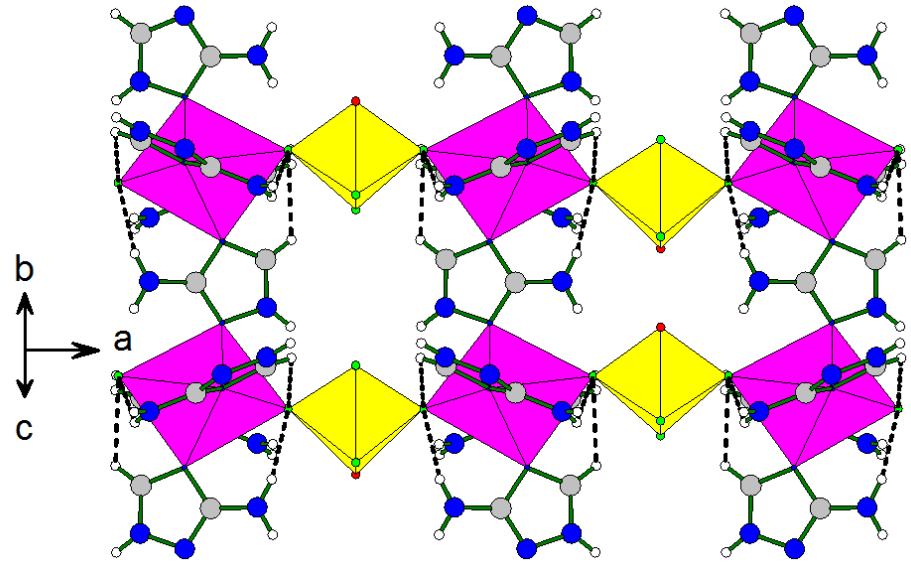

Fig. S4. Hydrogen bonds.

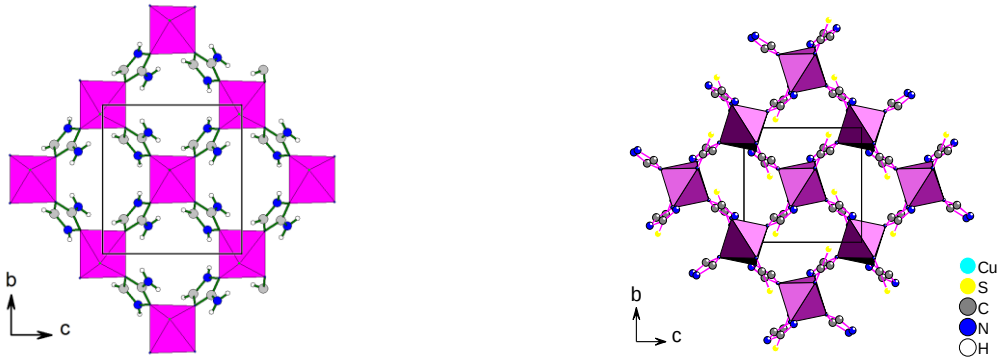

Fig. S5. Layer of $CuAlF_5(H_2O)[HAmTAZ]_2$ (left) and $Cu(TAZ)_2(NCS)_2$ (right). Hydrogens are omitted for clarity.

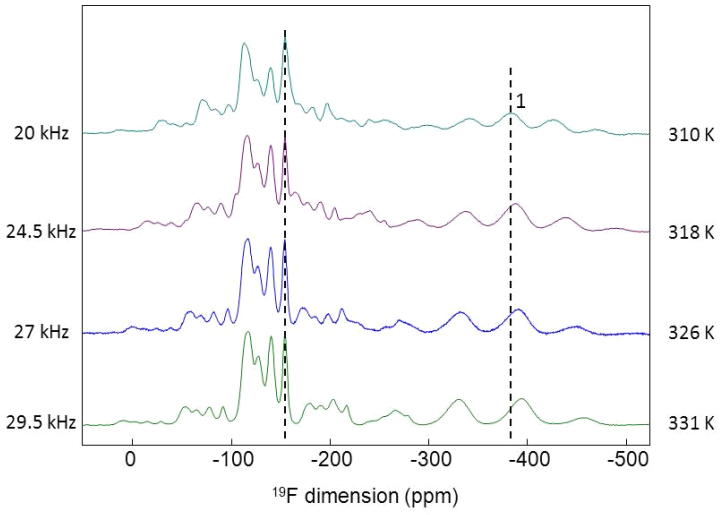

Fig. S6. 19F MAS NMR spectra of $CuAlF_{4.5}(OH)_{0.5}(H_2O)[HAmTAZ]_2$ recorded at various MAS frequencies. The dash lines are a guide for the eye. Temperature of the sample at these MAS frequencies was calibrated using the 207Pb chemical shift in solid lead nitrate.

Table S2. ^{1}H and ^{19}F line label, line intensity (%), isotropic chemical shift δ_{iso} (ppm), chemical shift anisotropy δ_{CS} (ppm) and asymmetry parameter η_{CS} in $CuAlF_5(H_2O)[AmTAZ]_2$.

Line	Intensity (± 0.5)	δ_{iso} (± 0.5)	δ_{CS} (± 1)	η_{CS} (± 0.1)
		^{1}H		
1	42.1	1.9	100	0.0
2	39.3	12.5	95	0.8
3	18.6	45.5	107	0.5
		^{19}F		
1	31.7	-456.4		
2	11.9	-154.2	95	0.7
3	18.1	-140.3	107	0.4
4	15.8	-127.4	105	0.7
5	9.0	-118.8	93	0.9
6	13.5	-113.4	93	0.9

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