Electronic Supplementary Information for Dalton Transactions

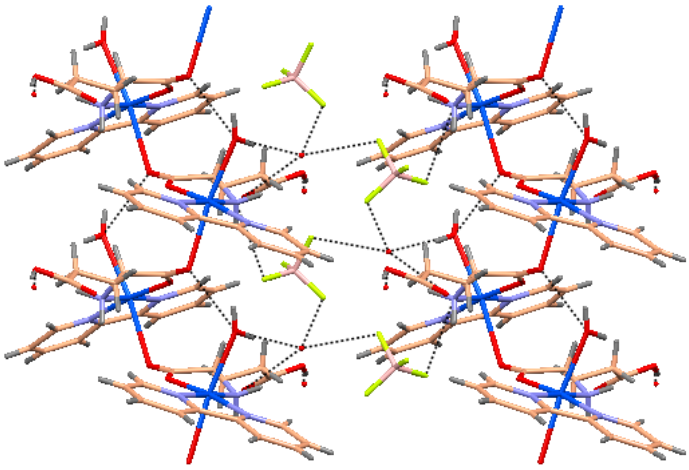

Figure S-1: Two-dimensional hydrogen-bonded architecture in **1**.

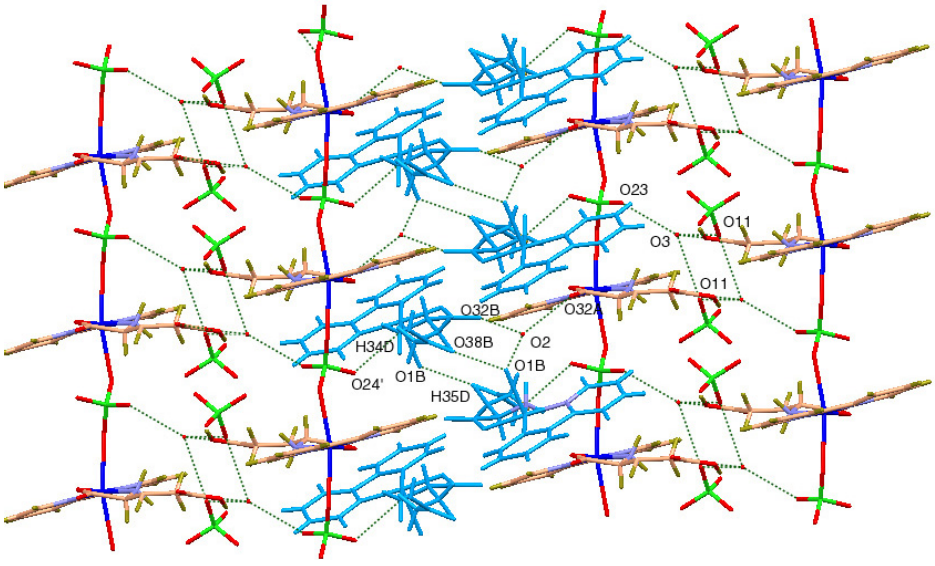

Figure S-2: Two-dimensional hydrogen-bonded sheet architecture in **2**.

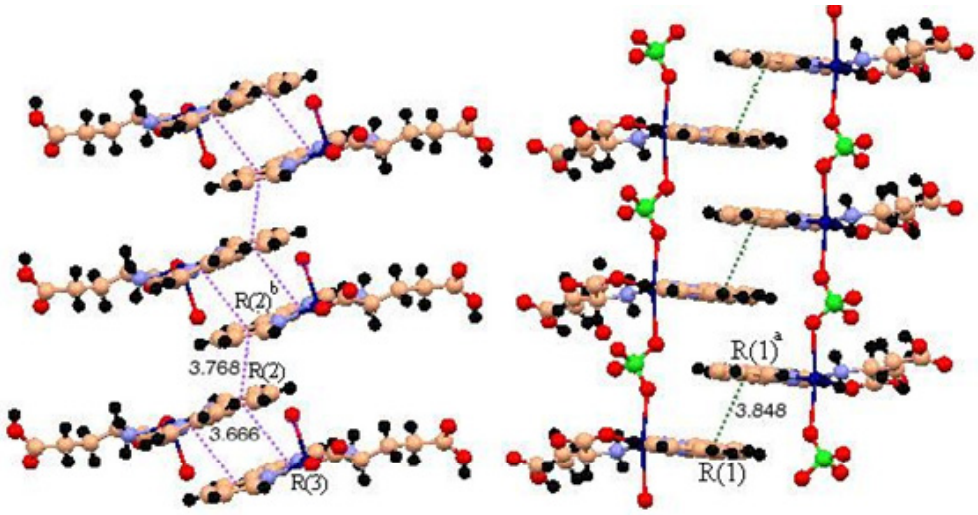

Figure S-3: Face-to-face π···π interactions (distances, Å) shown by magenta dotted lines for molecule **B** and green dotted lines for molecule **A** in complex **2.**

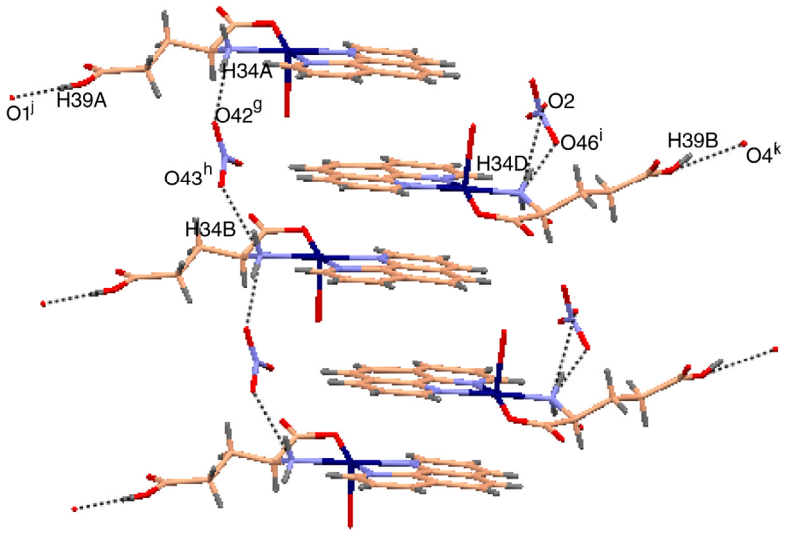

Figure S-4: Hydrogen-bonds and π···π interactions in **3**

Symmetry element ^{g} = 1+x,1+y,1+z, ^{h} = x,1+y,1+z, ^{i} = x,y,1+z, ^{j} = x,1+y,z, ^{k} = x,-1+y,z

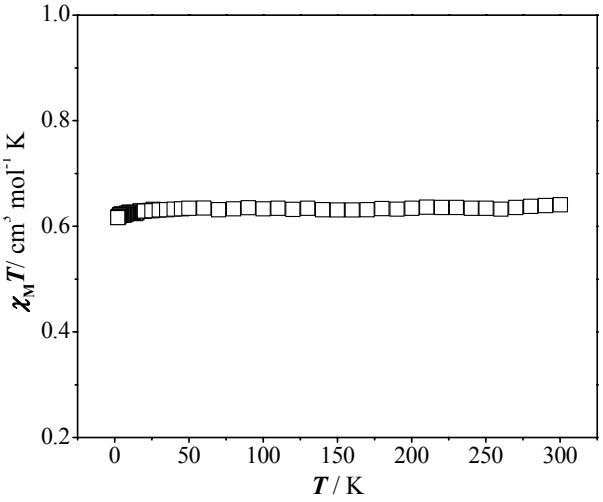

Figure S-5. Plot of $\chi_M T$ vs$T$ for complex **1**

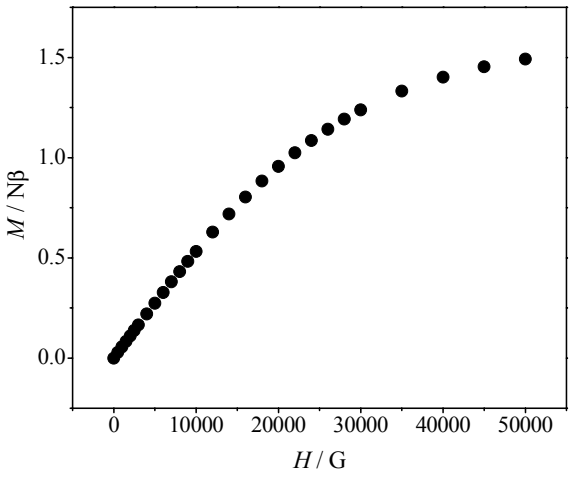

Figure S-6. Field dependence of the magnetization of complex **1** at 2 K

Table S-1: Hydrogen bonds (distances, Å, angles, deg) in the two structures Between D (donor) and A (acceptor)

D–H····A	d(D–H)	d(H····A)	d(D····A)	(∠D–H····A)
Complex 1				
N34 – H34A ··· O2	0.90	2.15	2.98(1)	153
N34 – H34B ··· F23[a]	0.90	2.19	3.01(1)	151
O39 – H39 ··· O3[b]	0.82	1.79	2.59(1)	167
O1 – HO1 ··· O2	0.86(1)	2.01(9)	2.85(1)	167(1)
O1 – HO2 ··· O32[c]	0.85(3)	2.28(9)	2.87(1)	127(9)
Complex 2				
N34A – H34A ··· O3[d]	0.90	2.37	3.19(6)	152
N34A–H34B ··· O11[d]	0.90	2.48	3.19(5)	137
N34B–H34C···O31A[e]	0.90	2.40	3.21(5)	148
N34B – H34D ··· O2[f]	0.90	2.34	3.17(6)	153
N34B–H34D ··· O24[e]	0.90	2.51	2.30(6)	114
O39A – H39A ··· O3	0.82	1.98	2.69(5)	144
Complex 3				
N34A–H34A···O42[g]	0.90	2.23	3.12(2)	170
N34A–H34B ··· O43[h]	0.90	2.14	3.02(2)	163
N34B–H34C ··· O3[i]	0.90	2.13	2.97(2)	155
N34B–H34D ··· O2	0.90	2.22	3.09(2)	162
N34B–H34D ··· O46[j]	0.90	2.59	3.21(2)	126
O39A–H39A ··· O5[k]	0.82	1.69	2.49(2)	165
O39B–H39B ··· O4[l]	0.82	1.89	2.66(1)	157

Symmetry operators: [a]= 0.5-x, 0.5+y, 0.5-z, [b]= 0.5-x, -0.5+y, 0.5-z, [c]= -0.5-x, -0.5+y, 0.5-z, [d]= 1- x, -1-y, 2-z, [e] = x, 1+y, z, [f]= 1+x, y, z, [g] = 1+x, 1+y, 1+z, [h] = x, 1+y, 1+z, [i] = x, -1+y, -1+z, [j] = x, y, 1+z, [k] = x, 1+y, z, [l] = x, -1+y, z

Table S-2. π—π Interactions (Face-to-Face) in Complex 1 and 2

Complex	Ring (i) → ring (j)	dihedral angle (i,j) (°)	slip angle (i,j) (°)	distance of centroid (i) from ring (j) (Å)	distance between the (i,j) ring centroids (Å)
1	R (1) → R(4)	6.90	21.62	3.238	3.664
	R (2) → R(3)	4.22	28.05	3.286	3.872
2	R(1) → R(1)[a]	0.00*	20.80	3.597	3.848
	R(2) → R(2)[b]	0.00[*]	31.25	3.221	3.767
	R(3) → R(2)[c]	10.82	26.67	3.276	3.666
3	R(1) → R(5)	1.56	17.24	3.302	3.437
	R(2) → R(4)	2.80	16.47	3.294	3.456
	R(2) → R(6)[d]	12.7	1.10	3.308	3.582

Symmetry element [a] = 1-x,-y,2-z, [b] = 1-x,1-y,1-z, [c] = 2-x,1-y,1-z , [d] = 1+x, y, z

- Fixed at 0.00° across a centre of symmetry