Hydrogen bonding *versus* π–stacking in ferromagnetic interactions. Studies on a copper triazolopyridine complex

Carmen Ramírez de Arellano[a*], Emilio Escrivà[b], Carlos J. Gómez-García[c], Guillermo Mínguez Espallargas[c], Rafael Ballesteros[a] and Belén Abarca[a]

[a]*Departament de Química Orgànica,, Universitat de València, c/ Vicent Andrés Estellés, s/n, 46100 Burjassot (València) Spain.*
[b]*Departament de Química Orgànica, Universitat de València, c/ Vicent Andrés Estellés, s/n, 46100 Burjassot (València) Spain.*
[c]*Instituto de Ciencia Molecular (ICMol), Parque Científico, Universidad de Valencia, C/Catedrático José Beltrán, 2, 46980 Paterna, Valencia, Spain*

Supplementary information

Table 1. Hydrogen bonds for **[Cu(BTP)(H$_2$O)$_2$(BF$_4$)](BF$_4$)·2H$_2$O** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
1. Interactions within linear chains formed through OH$_2$···F$_4$B				
O(2)-H(04)...F(8')#3	0.68(3)	2.23(3)	2.887(17)	162(6)
O(2)-H(04)...F(6')#3	0.68(3)	2.38(4)	2.967(8)	145(6)
O(2)-H(04)...F(8)#3	0.68(3)	2.58(4)	3.144(13)	143(6)
O(2)-H(04)...F(6)#3	0.68(3)	2.64(3)	3.288(12)	160(6)
2. Other interactions involved in the 3-D network				
2.1 Interactions of the coordinated water molecule (O1) with non coordinating water molecules (O98 and O99)				
O(1)-H(01)...O(99)	0.72(2)	1.92(2)	2.641(4)	179(4)
O(1)-H(02)...O(98)#1	0.69(3)	1.96(3)	2.632(4)	163(6)
2.2 Interaction of the coordinated water molecule (O2) with BF$_4^-$ anion				
O(2)-H(03)...F(1)#2	0.70(3)	2.16(3)	2.838(5)	165(5)
O(2)-H(03)...F(1')#2	0.70(3)	2.16(3)	2.776(6)	148(5)
2.3 Interactions of crystallization water molecules (O98 and O99) with BF$_4^-$ anions				
O(98)-H(06)...F(7)	0.86(3)	1.95(3)	2.760(5)	156(4)
O(98)-H(06)...F(5)	0.86(3)	3.24(4)	3.948(14)	142(4)
O(99)-H(07)...F(6)	0.83(2)	1.94(3)	2.747(12)	164(4)
O(99)-H(07)...F(8')	0.83(2)	1.99(3)	2.778(16)	158(4)
O(99)-H(08)...F(2')#4	0.85(3)	1.97(3)	2.804(6)	167(4)
O(99)-H(08)...F(4)#4	0.85(3)	2.14(3)	2.841(6)	140(4)
O(99)-H(08)...F(3)#4	0.85(3)	2.27(3)	3.040(6)	151(4)

Symmetry transformations used to generate equivalent atoms: #1 x+1/2,-y+1/2,z-1/2; #2 x,y,z-1; #3 x-1/2,-y+1/2,z-1/2; #4 -x+2,-y,-z+1.

Figure 1. Ellipsoids plot (50% probability level) for **[Cu(BTP)(H_2O)$_2$(BF_4)](BF_4)·2H_2O**.