Electronic Supplementary Material for CrystEngComm

Supplementary material for

Cation and ligand roles in the coordination of FeIII bisdithiolene complexes; The crystal structures of BrBzPy [Fe(qdt)$_2$] and [Fe(α-tpdt)$_2$] salts, by Ana Isabel Soares Neves, Isabel Cordeiro Santos, Dulce Belo and Manuel Almeida.

Table S1: Short contacts and hydrogen bonds in the crystal structure of BrBzPy[Fe(qdt)$_2$] (**1**)

	Interactions	Symmetry Op. contacting atom	d (Å)	Angle(º)
Fe1···S3^1	DD	2-x,-y,1-z	3.824	
C11···C1^2	DD	2-x,-y,1-z	3.292	
C15···C3^2	DD	2-x,-y,1-z	3.262	
S1···C9^2	DD	2-x,-y,1-z	3.529	
S2···C10^1	inD	-x,-y,-z	3.432	
Br1···C7^3	CA	1+x, y,-1+z	3.534	
Br1···H15-C15^4	CA	1-x, -y ,-z	3.043	137
N1···H27-C27^5	CA	2-x,1-y,1-z	2.697	118
N1···H28-C28^5	CA	2-x,1-y,1-z	2.503	128
N2···H25-C25^6	CA	1-x, -y, 1-z	2.519	172
N3···H24-C24^7	CA	x, y, z	2.345	118
S1···H21-C21^5	CA	2-x,1-y,1-z	2.959	155
S2···H17-C17^5	CA	2-x,1-y,1-z	2.958	165
S3···H20-C205	CA	2-x,1-y,1-z	3.373	150
S4···H21-C21^8	CA	1+x,1+y, z	2.884	116
C19-H19···C25^5	CC	2-x,1-y,1-z	2.876	145
C19-H19···C26^5	CC	2-x,1-y,1-z	2.810	169
C19-H19···C27^5	CC	2-x,1-y,1-z	2.870	163

D= dimmer, inD=intradimmer, C=cation and A=anion

Table S2: Short contacts and hydrogen bonds in the crystal structure of BrBzPy[Fe(α-tpdt)$_2$] (**2**)

	Interactions	Symmetry Op. contacting atom	d (Å)	Angle(º)
Br1···C16	CC	x, ½ -y, ½ +z	3.380	
C16···H11	CC	1-x, 1-y, -z	2.850	
C17···H11	CC	1-x, 1-y, -z	2.822	
S2···C13	CA	1-x, 1-y, 1-z	3.473	
Br1···H8-C8	CA	1-x, 1-y, z	3.017	139°
S1···H10-C10	CA	-x, 1-y, z	2.811	156°
S2···H12-C12	CA	1-x, 1-y, 1-z	2.923	120°
S2···H13-C13	CA	1-x, 1-y, 1-z	2.861	123°
S2···H14b-C14	CA	x, y, z	2.941	142°
S5···H13-C13	CA	1-x, 1-y, 1-z	2.897	156°
S6···H16-C16	CA	-x, 1.y, -z	2.982	136°

C=cation and A=anion