Electronic Supplementary Material (ESI) for Dalton Transactions

New series of hybrid fluoroferrates synthesized with triazoles: various dimensionalities and magnetic properties

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SUPPLEMENTARY INFORMATION

Figure S1. Composition space of the FeF_2-FeF_3-H*taz*-$HF_{aq.}$-DMF system established under solvothermal conditions (120°C, 72 h) for a constant concentration $[Fe^{II}]+[Fe^{III}]$ = 0.15 mol.L^{-1} and a ratio $[Fe^{II}]/[Fe^{III}]$ = 1.

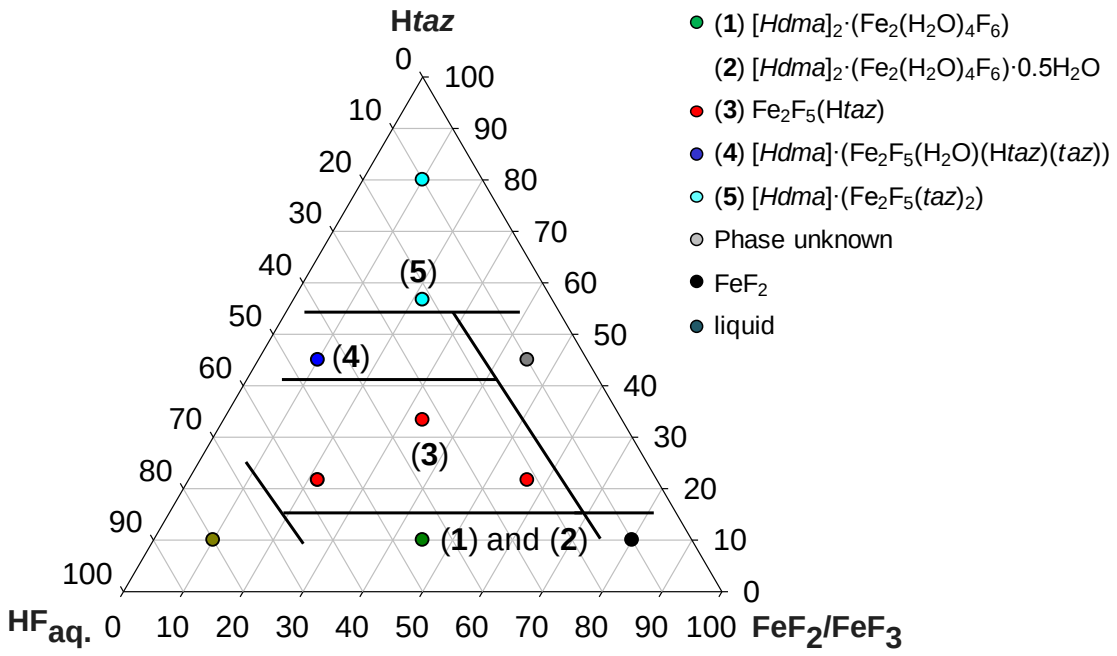

Figure S2. Diagram pattern obtained in the FeF_2-FeF_3-H*taz*-$HF_{aq.}$-DMF system with a 2/2/1/2/323 molar ratio : (1) and (2)

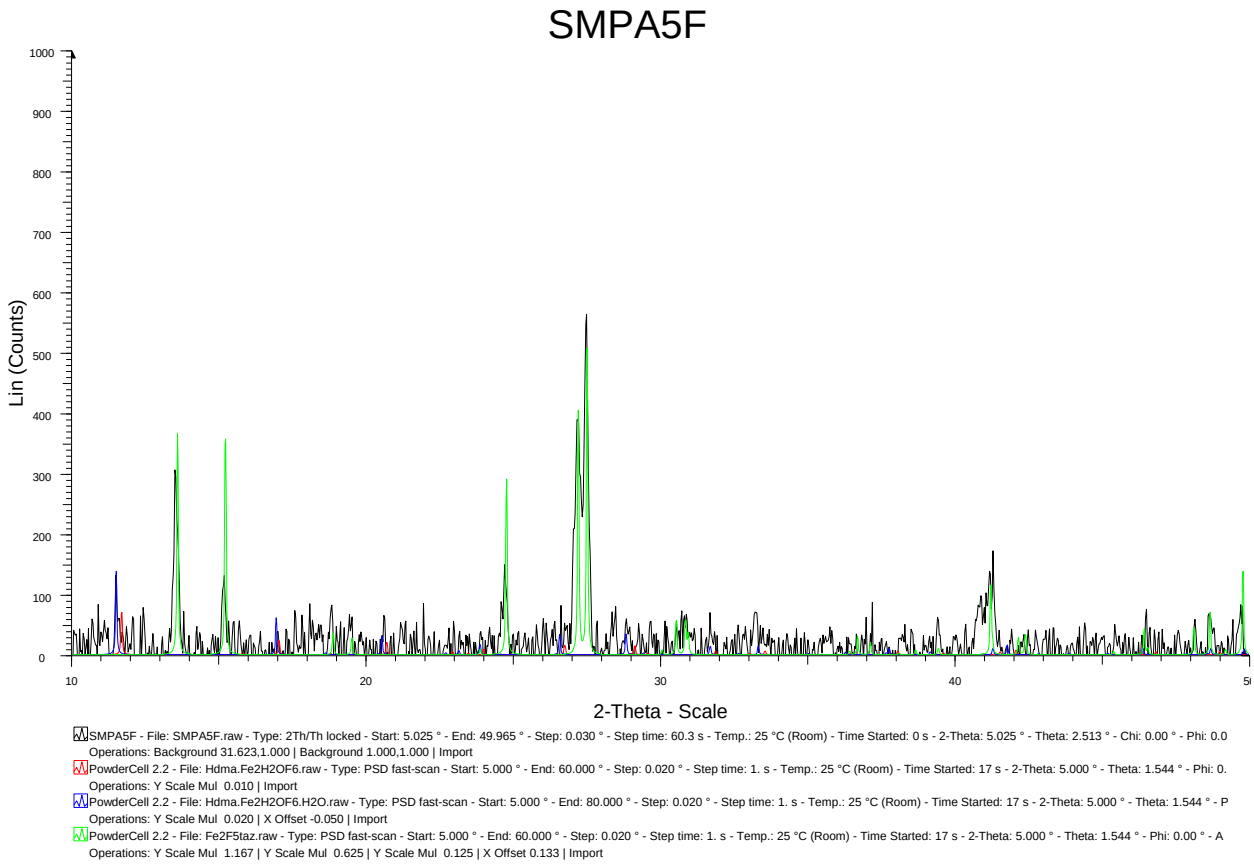

Figure S3. Diagram pattern obtained in the FeF_2-FeF_3-H*taz*-$HF_{aq.}$-DMF system with a 2/2/17/17/323 molar ratio (4)

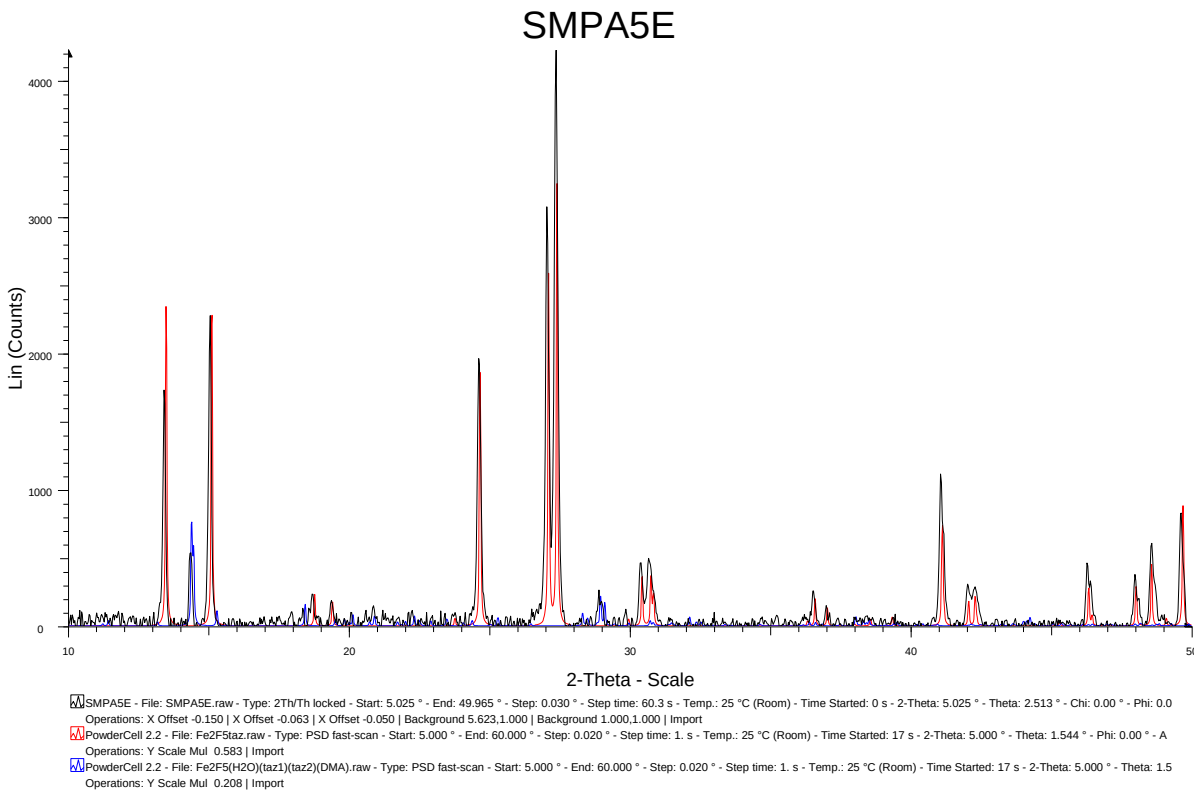

Figure S4. Diagram pattern obtained in the FeF_2/FeF_3-H*taz*-$HF_{aq.}$-DMF system with a 2/2/10/4/323 molar ratio (5)

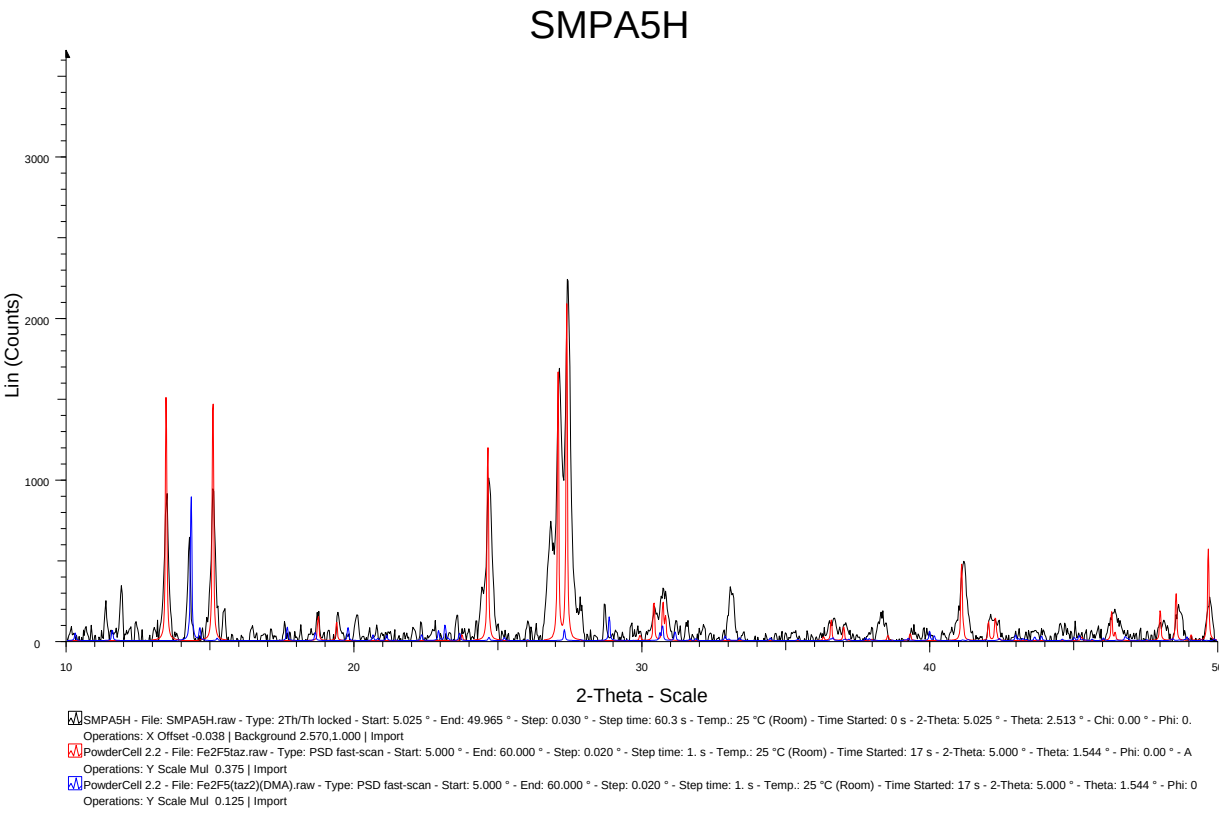

Table S1. Atomic coordinates and equivalent APD of [H*dma*]·($Fe_2(H_2O)_4F_6$) (1)

Atom	Wyckoff position	x	Y	z	B_{eq}(Å^2)
Fe(1)	4a	½	½	½	1,29(2)
Fe(2)	4b	½	1	½	1,29(2)
F(1)	8f	½	0.7570(2)	0.54882(17)	1,86(5)
F(2)	16h	0.63082(15	0.9287(2)	0.41707(11)	2,15(3)
OW(1)	16h	0.36125(18	0.4262(2)	0.59871(14)	1,95(4)
C(1)	8g	0.3813(7)	0.7462(6)	¾	3,79(11)
N(1)	4c	½	0.6359(7)	¾	2,88(9)

Table S2. Atomic coordinates and equivalent APD of [H*dma*]·($Fe_2(H_2O)_4F_6$)·0.5H_2O (2)

Atom	Wyckoff position	x	y	z	B_{eq}(Å^2)
Fe(1)	4a	½	½	½	1,34(2)
Fe(2)	4b	½	1	½	1,27(2)
F(1)	8f	½	0.7570(2)	0.54779(17)	1,82(4)
F(2)	16h	0.63035(16)	0.9294(2)	0.41655(12)	2,30(4)
OW(1)	16h	0.36143(18)	0.4269(3)	0.59472(14)	2,07(4)
C(1)	8g	0.3826(7)	0.7331(8)	¾	4,02(12)
N(1)	4c	½	0.61587(7)	¾	4,03(14)
OW(2)	4c	0	0.7109(8)	¾	5,52(40)

Table S3. Atomic coordinates and equivalent APD of Fe_2F_5(H*taz*) (3)

Atom	Wyckoff position	x	y	z	B_{eq}(Å^2)
Fe(1)	4a	½	½	½	1,10(8)
Fe(2)	4c	¾	¾	¾	1,67(8)
F(1)	4e	½	¾	0.4318(5)	1,11(2)
F(2)	16j	0.6461(3)	0.5537(4)	0.6367(2)	1,56(1)
N(1)	8i	0.9258(5)	¾	0.5845(6)	1,74(3)
N(2)	4e	1	¾	0.3695(7)	1,74(3)
C(1)	8i	0.8845(7)	¾	0.4590(9)	3,47(4)

Table S4. Atomic coordinates and equivalent APD of [H*dma*]·($Fe_2F_5(H_2O)$(H*taz*)(*taz*)) (4)

Atom	Wyckoff position	x	y	z	B_{eq}(Å^2)
Fe(1)	2i	0.32425(7)	0.27136(6)	0.38112(6)	1,24(15)
Fe(2)	1a	0.0000	0.0000	0.0000	1,12(2)
Fe(3)	1e	0.5000	0.5000	0.0000	1,22(2)
F(1)	2i	0.4751(3)	0.4337(2)	0.2221(2)	1,76(4)
F(2)	2i	0.1494(3)	0.4150(3)	0.4347(3)	2,05(5)
F(3)	2i	0.3709(3)	0.3357(3)	0.5416(3)	2,17(5)
F(4)	2i	0.1617(3)	0.1213(2)	0.5193(2)	1,95(4)
F(5)	2i	0.5015(3)	0.1403(3)	0.3306(3)	2,31(5)
O(1)	2i	0.2102(4)	0.0119(3)	-0.2356(3)	2,06(6)
N(6)	2i	0.0976(4)	0.8035(4)	0.0830(4)	1,52(6)
N(1)	2i	0.2656(4)	0.2266(4)	0.1986(4)	1,56(6)
N(2)	2i	0.1536(4)	0.1337(4)	0.0614(4)	1,67(6)
N(3)	2i	0.3285(4)	0.3105(4)	0.0520(4)	1,57(6)
N(4)	2i	0.2846(4)	0.6418(4)	0.0915(4)	1,88(6)
N(5)	2i	0.1320(4)	0.6079(4)	0.2177(4)	1,78(6)
N(7)	2i	0.3087(5)	0.6561(4)	0.5018(5)	3,45(9)
C(1)	2i	0.1631(5)	0.1239(4)	0.1982(4)	1,68(7)
C(2)	2i	0.2590(5)	0.2503(4)	-0.0243(5)	1,80(7)
C(3)	2i	0.0240(5)	0.7056(4)	0.2111(4)	1,65(7)
C(4)	2i	0.2583(4)	0.7608(3)	0.0132(3)	1,97(8)
C(5)	2i	0.2947(4)	0.7963(3)	0.4075(3)	5,09(14)
C(6)	2i	0.2019(4)	0.6460(3)	0.6726(3)	4,43(12)

Table S5. Atomic coordinates and equivalent APD of [H*dma*]·($Fe_2F_5(taz)_2$) (5)

Atom	Wyckoff position	x	y	z	B_{eq}(Å^2)
Fe(1)	4c	0.42845(7)	¼	0.31073(15)	1,64(3)
Fe(2)	4c	0.22819(7)	¼	0.24328(16)	1,25(2)
F(1)	4c	0.4961(3)	¼	0.4773(7)	3,15(13)
F(2)	4c	0.3368(3)	¼	0.1618(6)	1,85(9)
F(3)	8d	0.4739(2)	0.4041(4)	0.1949(5)	3,11(9)
F(4)	4c	0.1316(3)	¼	0.3356(6)	2,89(12)
N(1)	8d	0.2256(3)	-0.0909(6)	-0.0997(6)	1,73(9)
N(2)	8d	0.1464(3)	-0.0892(6)	-0.0683(6)	1,73(9)
N(3)	8d	0.2033(3)	0.0805(6)	0.0811(6)	1,66(9)
C(1)	8d	0.1362(4)	0.0140(7)	0.0400(7)	1,62(11)
C(2)	8d	0.2573(3)	0.0127(7)	-0.0078(6)	1,58(11)
C(4)	4c	0.4012(3)	¾	0.1994(6)	3,80(2)
C(3)	4c	0.5386(3)	¾	0.1466(6)	4,12(2)
N(4)	4c	0.4624(3)	¾	0.1006(6)	13,2(8)

Table S6. Selected H-bond, D-H··· A (D = N, O ; A = F, O) distances (Å) in [H*dma*]·($Fe_2(H_2O)_4F_6$) (1), [H*dma*]·($Fe_2(H_2O)_4F_6$)·0.5H_2O (2), [H*dma*]·(Fe_2F_5(H*taz*)(*taz*)) (4) and [H*dma*]·($Fe_2F_5(taz)_2$) (5)

D-H···A	d(D···A)
(**1**)	
OW(1)-H(1)WA···F(2)	2.644(3)
OW(1)-H(1) WB···F(2)	2.639(3)
N(1)-H(1)A··· OW(1) x2	3.123(4)
N(1)-H(1)B···OW(1) x2	3.123(4)
(**2**)	
OW(1)-H(1)WA···F(2)	2.642(3)
OW(1)-H(1) WB···F(2)	2.655(3)
N(1)-H(1)A··· OW(1) x2	3.128(4)
N(1)-H(1)B···OW(1) x2	3.128(4)
(**3**)	
N(5)-H(5)···F(2)	2.599 (5)
N(7)-H(7)A···F(2)	2.932(6)
N(7)-H(7)A···F(3)	2.993(5)
N(7)-H(7)B···F(3)	2.674(6)
(4)	
N(4)-H(4)A···F(3) x 2	3.079(8)
N(4)-H(4)A···F(4)	2.779(8)

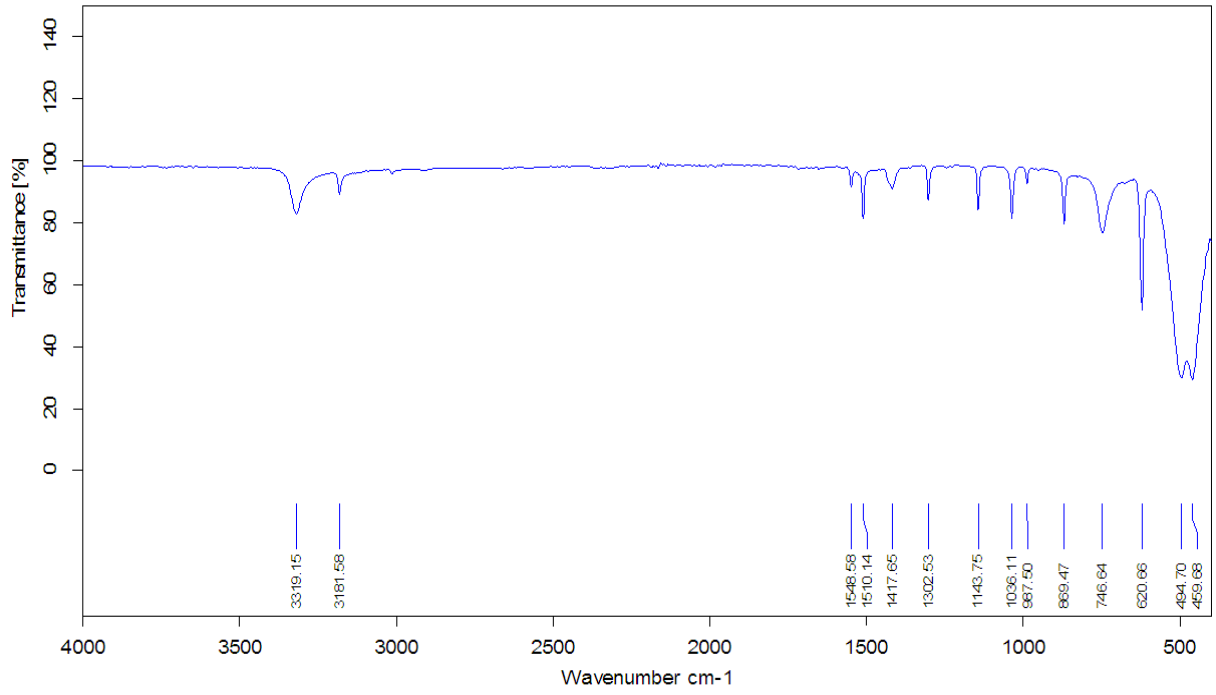

Figure S5. Infrared spectroscopy de Fe_2F_5(H*taz*)