Supporting information

Table S1. Selected hydrogen bonds lengths [Å] and angles [°] for **1-10**.

Donor-H···Acceptor	D-H	H···A	D···A	D-H···A
		1		
O1-H1A ···S1[a]	0.84	2.37	3.2032	169
O1-H1B···N2[b]	0.84	1.96	2.7943	172
		2		
O1W-H1A···N5[a]	0.85	2.16	3.0031	173
O1W-H1B···N5[b]	0.85	2.15	2.9921	170
C2 -H9···S1[c]	0.93	2.70	3.6206	171
		3		
O1-H1A··· N8[a]	0.84	1.95	2.7912	177
O1-H1B···Cl2[b]	0.84	2.27	3.1000	171
O2-H2A···Cl2[c]	0.84	2.27	3.1049	171
O2-H2B···N7[a]	0.84	1.98	2.816	177
O3 -H3A ···Cl2	0.84	2.45	3.2844	173
O3--H3B···Cl1[d]	0.84	2.48	3.2623	156
C3-H3···O3[e]	0.95	2.43	3.107	128
C4-H4···Cl2[f]	0.95	2.79	3.5844	141
C4-H4···O3[g]	0.95	2.49	3.160	128
		4		
O1-H1 ···N12[a]	0.85	1.91	2.7528	173
O1-H1B···O3	0.85	1.82	2.6553	166
O2-H2A ···Br1	0.85	2.43	3.2720	175
O2-H2B···Br1[b]	0.85	2.47	3.3192	178
O3-H3A ···O2[c]	0.85	1.88	2.7231	170
O3-H3B···N11[d]	0.85	2.04	2.8746	166
C2-H2···O3[e]	0.93	2.36	3.2337	157
		5		
O1W-H1A···N7[a]	0.85	1.99	2.8129	162
O1W-H1B···O2W	0.85	1.85	2.6894	169
O2W-H2A···N8[b]	0.85	2.06	2.9043	171
O2W-H2B···F4[c]	0.85	2.08	2.8502	150
C1-H1···N10	0.9300	2.61	3.1360	117
C2-H2···F3[d]	0.9300	2.34	3.1956	153
C4-H4 ···F2	0.9300	2.34	3.2145	157
C5-H5 ···O2W[e]	0.9300	2.46	3.3704	166
C6-H6···F4	0.9300	2.49	3.2331	137

6				
C3-H3···N6[a]	0.93	2.52	3.0927	120
C4-H4···N3[b]	0.93	2.60	3.1544	118
C5-H5···F2[c]	0.93	2.36	3.2906	176
C6-H6···F2[d]	0.93	2.39	3.3026	169
7				
O1-H1A···F4[a]	0.85	2.06	2.8935	166
O1-H1B···.F1	0.85	2.35	3.1849	168
O1-H1B···F2	0.85	2.45	3.0312	126
C2-H2···O1	0.95	2.41	3.2951	154
C3-H3···F1[b]	0.95	2.39	3.2360	148
C4-H4···F1	0.95	2.54	3.4073	152
C4-H4···F3	0.95	2.53	3.3788	149
C5-H5···N3[c]	0.95	2.62	3.0894	111
C5-H5···N7[d]	0.95	2.60	3.1281	115
C6-H6···N11[e]	0.95	2.47	3.0819	122
8				
O5-H5A···O11[a]	0.85	1.97	2.7470	151
O5-H5B···O2[b]	0.85	1.92	2.7263	159
O6-H6A···O14	0.85	2.04	2.7865	146
O6-H6B···O12	0.85	1.88	2.7249	170
O7-H7···O4[b]	0.85	1.97	2.7985	165
O8-H8A···O1[b]	0.85	1.93	2.7462	160
O8-H8B···O5[c]	0.85	1.98	2.7852	158
O9-H9A···O6	0.85	1.95	2.7842	166
O9-H9B···O3[d]	0.85	1.90	2.7009	157
O10-H10···O3[a]	0.85	1.96	2.8062	174
O11-H11A···O7	0.85	2.05	2.8796	165
O11-H11B···O8[e]	0.85	1.94	2.7544	161
O12-H12A···O10[e]	0.85	2.04	2.8892	173
O12-H12B···O9[f]	0.85	2.05	2.7716	142
O13-H13A···O4[a]	0.85	2.25	2.9399	139
O13-H13B···O2	0.85	2.01	2.8018	155
O14-H14A···O2[a]	0.85	1.99	2.8356	171
O14-H14B···O1[d]	0.85	1.93	2.7821	175
C1-H1···O11	0.93	2.32	2.9861	128
C1-H1···O4[b]	0.93	2.43	2.9213	113
C2-H2···O4[g]	0.93	2.16	2.9588	143
C3-H3···O13[e]	0.93	2.16	2.9765	146
C4-H4···O13[a]	0.93	2.27	3.1086	150
9				
C2-H2···N2	0.95	2.56	3.3343	139
10				

C1-H1···N6[a]	0.93	2.34	3.2110	156
C2-H2···O1	0.93	2.22	3.1477	173
C2-H2···O1[b]	0.93	2.52	2.9173	106
C4-H4···N2[c]	0.93	2.33	3.2328	165

Symmetry codes: For **1**: a: -1+x,y,z ; b: 1-x,1-y,1-z. For **2**: a: x,1-y,-1/2+z; b: 1/2-x,1/2-y,-z; c: 1/2-x,-1/2+y,1/2-z. For **3**: a: 1-x,2-y,1-z; b: 1+x,1+y,z; c: x,1+y,z; d: 1-x,-1/2+y,1/2-z; e: 1-x,1-y,1-z; f: -x,1/2+y,1/2-z; g: -x,1-y,1-z. For **4**: a: -1+x,y,1+z; b: 2-x,1-y,-z; c: -1+x,y,z; d: 1-x,1-y,-z; e: x,-1+y,z. For **5:** a: x,y,1+z; b: 1-x,-y,-z; c: -1+x,y,z; d: 1-x,1-y,-z; e: 1-x,-y,1-z. For **6:** a: 1-x,1-y,-z; b: 1-x,-y,-z; c: -x,1-y,1-z; d: 1-x,1-y,1-z. For **7**: a: 1/2+x,1/2-y,1/2+z; b: 1+x,y,z; c: 2-x,-y,-z; d: 1/2+x,1/2-y,-1/2+z; e: 2-x,-y,1-z. For**8**: a: -1+x,y,z; b: -1+x,1-y,1/2+z; c: x,1+y,z; d: -1+x,1+y,z; e: 1+x,y,z; f: x,-1+y,z; g: -1+x,-y,1/2+z. For **10**: a: x,1+y,z; b: 1-x,1-y,1-z; c: 1-x,2-y,-z.

Table S2 Dihedral angles of between two triazole rings of atrz for **1-10**

	Dihedral angles between two triazole rings of atrz (°)
1	0 °
2	0 °
3	2.41(6)°
4	0 ° and 12.45(8)°
5	0 ° and 6.77(0)°
6	0 ° and 18.03(1)°
7	0 °
8	5.45(9) °
9	0 °
10	0 °

Table S3 Selected Bond Lengths (Å) and Angles (°) for **1-10**

1					
Fe(1)-O(1)	2.1049(15)	Fe(1)-O(1A)	2.1049(15)	Fe(1)-N(5A)	2.1375(17)
Fe(1)-N(5)	2.1375(17)	Fe(1)-N(1A)	2.2030(17)	Fe(1)-N(1)	2.2031(17)
O(1A) -Fe(1)-N(5)	89.77(6)	O(1)-Fe(1)-N(5)	90.23(6)	O(1)-Fe(1)-N(1)	86.80(6)
N(5A) -Fe(1)-N(5)	179.999(1)	O(1)-Fe(1)-N(1A)	93.20(6)	N(5)-Fe(1)-N(1)	87.00(7)
O(1)-Fe(1)-O(1A)	180.0	O(1A) -Fe(1)-N(1A)	86.80(6)	N(1A) -Fe(1)-N(1)	180.00(8)
2					
Fe(1)-O(1)	2.108(2)	Fe(1)-N(1A)	2.115(2)	Fe(1)-N(1)	2.115(2)
Fe(1)-O(1A)	2.108(2)	Fe(1)-N(4A)	2.223(2)	Fe(1)-N(4)	2.223(2)
O(1A) -Fe(1)-N(1)	90.23(9)	O(1)-Fe(1)-N(1)	89.77(9)	N(1A) -Fe(1)-N(1)	180.00(11)
N(1)-Fe(1)-N(4A)	88.29(9)	O(1)-Fe(1)-N(4A)	89.47(8)	N(1)-Fe(1)-N(4)	91.71(9)
O(1)-Fe(1)-O(1A)	180.0	O(1)-Fe(1)-N(4)	90.53(8)	N(4A)-Fe(1)-N(4)	180.0
3					
Fe(1)-O(1)	2.0791(13)	Fe(1)-O(1A)	2.0791(13)	Fe(1)-N(3B)	2.2162(15)
Fe(1)-N(3C)	2.2162(15)	Fe(1)-Cl(1A)	2.4865(4)	Fe(1)-Cl(1)	2.4865(4)
Fe(2)-O(2)	2.0869(13)	Fe(2)-O(2C)	2.0869(13)	Fe(2)-N(2)	2.2006(15)
Fe(2)-N(2C)	2.2006(15)	Fe(2)-Cl(1)	2.4934(4)	Fe(2)-Cl(1C)	2.4934(4)
O(1)-Fe(1)-O(1A)	179.999(1)	O(1)-Fe(1)-Cl(1A)	90.65(4)	O(1)-Fe(1)-Cl(1)	89.34(4)
O(1A)-Fe(1)-Cl(1)	90.66(4)	N(3B)-Fe(1)-Cl(1)	90.98(4)	N(3C)-Fe(1)-Cl(1)	89.01(4)
Cl(1A)-Fe(1)-Cl(1)	180	O(1A)-Fe(1)-N(3C)	88.53(5)	O(1)-Fe(1)-N(3C)	91.48(5)
O(2)-Fe(2)-Cl(1)	89.36(4)	O(2C)-Fe(2)-Cl(1)	90.64(4)	N(2C)-Fe(2)-Cl(1)	88.83(4)
O(1A) -Fe(1)-N(3B)	91.47(5)	N(2)-Fe(2)-Cl(1)	91.17(4)	O(2)-Fe(2)-Cl(1C)	90.64(4)
N(2)-Fe(2)-Cl(1C)	88.83(4)	N(2C)-Fe(2)-Cl(1C)	91.17(4)	O(2C)-Fe(2)-Cl(1C)	89.36(4)
O(1)-Fe(1)-N(3B)	88.52(5)	O(2)-Fe(2)-O(2C)	180	Cl(1)-Fe(2)-Cl(1C)	180.0
4					
Fe(1)-O(1A)	2.0455(19)	Fe(1)-O(1)	2.0455(19)	Fe(1)-N(1)	2.189(2)
Fe(1)-N(1A)	2.189(2)	Fe(1)-N(5)	2.207(2)	Fe(1)-N(5A)	2.207(2)
N(1)-Fe(1)-N(5)	91.20(9)	O(1)-Fe(1)-N(1)	90.83(9)	N(1A)-Fe(1)-N(5)	88.80(9)
N(1)-Fe(1)-N(5A)	88.80(9)	O(1A)-Fe(1)-N(5)	89.03(8)	N(1A)-Fe(1)-N(5A)	91.20(9)
O(1A)-Fe(1)-O(1)	180.0	O(1)-Fe(1)-N(5)	90.97(8)	N(5)-Fe(1)-N(5A)	179.999(1)
5					
Fe(1)-O(1)	2.069(4)	Fe(1)-O(1A)	2.069(4)	Fe(1)-N(9A)	2.189(4)
Fe(1)-N(9)	2.189(4)	Fe(1)-N(1)	2.206(4)	Fe(1)-N(1A)	2.206(4)
O(1A)-Fe(1)-N(9)	91.26(15)	O(1)-Fe(1)-N(9)	88.74(15)	O(1)-Fe(1)-N(1A)	88.54(16)
N(9A)-Fe(1)-N(1)	90.96(15)	N(9)-Fe(1)-N(1)	89.04(15)	O(1)-Fe(1)-N(1)	91.46(16)
O(1)-Fe(1)-O(1A)	179.999(1)	O(1A)-Fe(1)-N(1)	88.54(16)	N(1)-Fe(1)-N(1A)	180.00(10)

6					
Cu(1)-N(5A)	2.020(3)	Cu(1)-N(5)	2.020(3)	Cu(1)-N(9A)	2.024(3)
Cu(1)-N(9)	2.024(3)	Cu(1)-N(2A)	2.423(4)	Cu(1)-N(2)	2.423(4)
N(9)-Cu(1)-N(2A)	89.11(15)	N(5A)-Cu(1)-N(9)	90.70(14)	N(5A)-Cu(1)-N(2)	89.77(14)
N(5)-Cu(1)-N(9)	89.30(14)	N(5)-Cu(1)-N(2)	90.23(14)	N(9)-Cu(1)-N(2)	90.89(15)
N(5A)-Cu(1)-N(5)	180.0	N(5)-Cu(1)-N(2A)	89.77(14)	N(2A)-Cu(1)-N(2)	180.0(2)
7					
Cu(1)-N(2A)	2.0134(16)	Cu(1)-N(2)	2.0134(16)	Cu(1)-N(10A)	2.0216(17)
Cu(1)-N(10)	2.0216(17)	Cu(1)-N(8B)	2.3896(16)	Cu(1)-N(8C)	2.3896(16)
N(2A)-Cu(1)-N(10)	91.31(6)	N(10)-Cu(1)-N(8B)	89.48(6)	N(10)-Cu(1)-N(8C)	90.51(6)
N(2)-Cu(1)-N(10)	88.69(6)	N(2)-Cu(1)-N(8C)	88.83(6)	N(2A)-Cu(1)-N(2)	180.00(8)
8					
Cu(1)-O(7)	1.940(4)	Cu(1)-O(10)	1.961(4)	Cu(1)-N(2A)	2.035(5)
Cu(1)-N(7B)	2.042(5)	Cu(1)-O(8)	2.437(5)	Cu(1)-O(9)	2.571(5)
Cu(2)-O(10C)	1.957(4)	Cu(2)-O(7)	1.956(4)	Cu(2)-N(3)	2.023(5)
Cu(2)-N(8B)	2.042(5)	Cu(2)-O(6)	2.463(5)	Cu(2)-O(10)	1.957(4)
O(7)-Cu(1)-O(8)	95.95(17)	O(10)-Cu(1)-O(8)	88.55(17)	O(8)-Cu(1)-O(9)	176.83(15)
N(2A)-Cu(1)-O(8)	85.97(18)	O(7)-Cu(1)-O(9)	84.80(16)	N(7B)-Cu(1)-O(9)	88.50(18)
O(10)-Cu(1)-O(9)	90.77(16)	O(7)-Cu(1)-O(10	175.4(2)	O(7)-Cu(2)-N(3)	92.94(18)
N(3)-Cu(2)-O(6)	94.85(19)	O(7)-Cu(2)-O(6)	87.49(16)	N(3)-Cu(2)-N(8B)	178.8(2)
9					
Zn(1)-N(5)	1.9314(15)	Zn(1)-N(5A)	1.9314(15)	Zn(1)-N(1)	2.0218(14)
Zn(1)-N(1A)	2.0218(14)	N(5)-Zn(1)-N(5A)	116.94(9)	N(5)-Zn(1)-N(1A)	119.47(6)
N(5)-Zn(1)-N(1)	99.27(6)	N(1)-Zn(1)-N(1A)	102.73(8)		
10					
Zn(1)-N(9)	1.923(2)	Zn(1)-N(5)	2.101(2)	Zn(1)-N(1)	2.0037(19)
Zn(1)-N(10)	1.930(2)	N(10)-Zn(1)-N(1)	109.13(10)	N(10)-Zn(1)-N(5)	100.54(9)
N(9)-Zn(1)-N(10)	127.71(11)	N(9)-Zn(1)-N(1)	116.03(9)	N(9)-Zn(1)-N(5)	98.61(9)

[a]Symmetry transformations used to generate equivalent atoms: For **1**: A -x+2,-y+1,-z+1. For **2**: A -x+1/2,-y+5/2,-z+1. For **3**: A -x+2,-y+2,-z; B x+1,y,z; C -x+1,-y+2,-z . For **4**: A -x,-y,-z+1. For **5**: A -x+1,-y+1,-z+1. For **6**: A -x+1,-y,-z. For **7**: A -x+2,-y,-z; B -x+3/2,y-1/2,-z+1/2 ; C x+1/2,-y+1/2,z-1/2. For **8**: A x,y+1,z; B x-1,-y+1,z-1/2; C x,y-1,z. For **9**: A -x+1,y,-z+1/2.

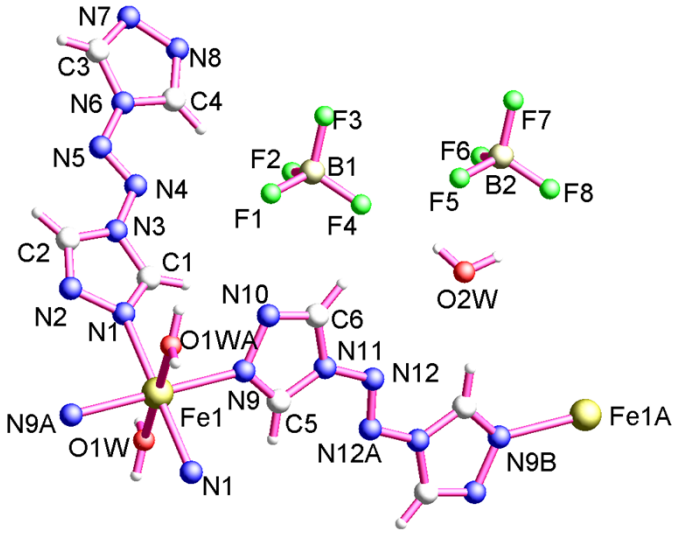

Fig. S1 The fundamental structural unit of $\{[Fe(\mu\text{-atrz})(atrz)_2(H_2O)_2]\cdot(BF_4)_2\cdot 2H_2O\}_n$ (**4**).

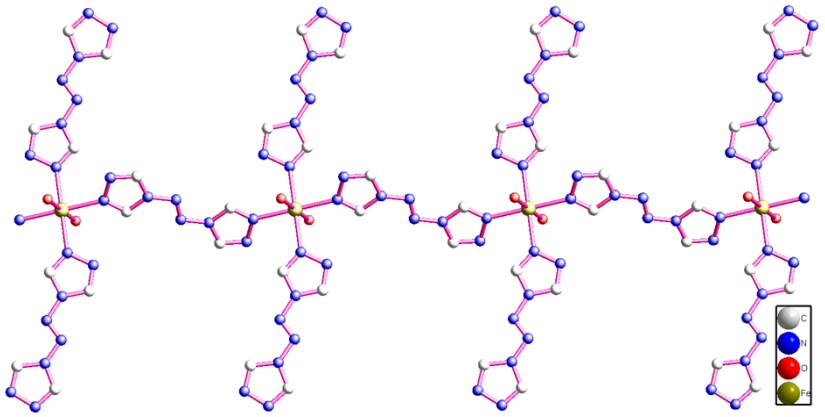

Fig. S2 The 1D iron(II)-triazole framework $\{[Fe(\mu\text{-atrz})(atrz)_2(H_2O)_2]\cdot(BF_4)_2\cdot 2H_2O\}_n$ (**4**).

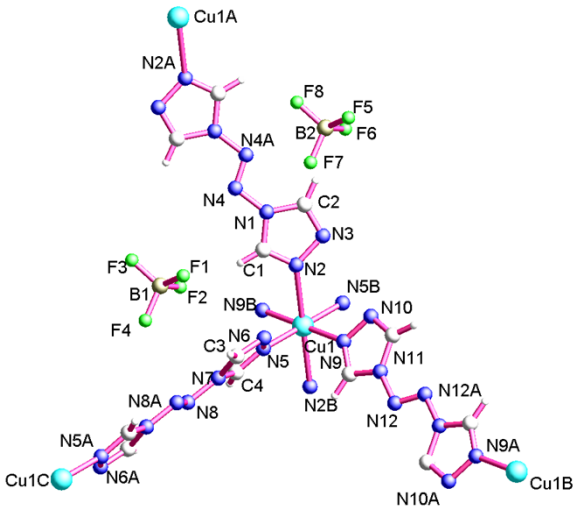

Fig. S3 The fundamental structural unit of $\{[Cu(\mu\text{-atrz})_3]\cdot(BF_4)_2\}_n$ (**6**).