A new hydrazone-linked covalent organic framework for Fe(III) detection by fluorescence and QCM technologies

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Supporting Information



Figure S1. (a) Experimental (red), simulated staggered stacking (blue), and simulated eclipsed stacking (black) PXRD patterns of Tfpa-Mth COF. (b) Eclipsed packing structure of Tfpa-Mth COF. (c) Staggered packing structure of Tfpa-Mth COF.



Figure S2. SEM image of Tfpa-Mth COF.



Figure S3. TEM image of Tfpa-Mth COF.



Figure S4. TGA curve of Tfpa-Mth COF.



Figure S5. Excitation (λ_{em} = 539 nm) and emission (λ_{ex} = 375 nm) spectra of Tfpa-Mth COF in

ethanol medium at room temperature.



Figure S6. Stern–Volmer plot of photoluminescent quenching efficiency (I_0/I) versus Fe³⁺ concentration in the Tfpa-Mth COF suspension (b) Linear relationship between Tfpa-Mth COF fluorescence intensity and Fe³⁺ concentration.



Figure S7. Fluorescence intensity changes of Tfpa-Mth COF at 539 nm in the presence of Fe³⁺ and other metal ions. The concentrations of all the metal ions were 1×10^{-4} M.



Figure S8. Fluorescence emission spectra of Tfpa-Mth COF suspension in various Fe^{3+} salt ethanol solutions (1×10⁻⁴ M).



Figure S9. The reusability of Tfpa-Mth COF for the detection of Fe³⁺ ion.



Figure S10. SEM image of the blank QCM chip. Inset: Cross-sectional view of the blank QCM chip.



Figure S11. FT-IR spectra of Tfpa-Mth COF and Tfpa-Mth COF@Fe³⁺.



Figure S12. PXRD patterns of Tfpa-Mth COF and Tfpa-Mth COF@Fe³⁺.



Figure S13. Zeta potential of Tfpa-Mth COF and Tfpa-Mth COF@Fe³⁺.



Figure S14. Fluorescence emission spectra of Tfpa before and after addition of Fe³⁺ ion in ethanol medium (λ_{ex} =370).

Tfpa-Mth COF with eclipsed packing			
Space group: P6 a = 39.63 Å, $b = 39.63$ Å, $c = 4.435$ Å $\alpha = \beta = 90^{\circ}, \gamma = 120^{\circ}$			
Atom	x/a	y/b	z/c
C1	1.587610	1.595640	0.690910
C2	1.607200	1.639920	0.638500
C3	1.579570	1.650300	0.467510
C4	1.646350	1.654140	0.477340
C5	1.597020	1.693980	0.412220
H6	1.693980	1.403190	1.608810
H7	1.666750	1.446460	1.591880
C8	1.525950	1.540730	0.851060
C9	1.540110	1.514450	0.860270
C10	1.530630	1.447490	0.886330

Table S1. Fractional atomic coordinates for the unit cell of Tfpa-Mth COF with eclipsed packing.

C11	1.514540	1.474050	0.866700
O12	1.516740	1.418120	0.731610
N13	1.560700	1.455450	1.078570
N14	1.575470	1.429880	1.099810
C15	1.603730	1.436380	1.281440
O16	1.550950	1.581460	0.840280
H17	1.607240	1.589800	0.832810
H18	1.583140	1.580760	0.469190
H19	1.613680	1.654710	0.860010
H20	1.552860	1.640700	0.604550
H21	1.570330	1.634460	0.250480
H22	1.642030	1.640190	0.253280
H23	1.665170	1.646580	0.613540
H24	1.662320	1.686270	0.451000
H25	1.620530	1.704570	0.240890
H26	1.608690	1.710490	0.625430
H27	1.574010	1.699620	0.325390
C28	1.650030	1.358730	1.323530
C29	1.600880	1.373620	1.141560
C30	1.616170	1.348660	1.155990
C31	1.667800	1.394330	1.480490
C32	1.652330	1.419190	1.469050
C33	1.618960	1.409230	1.297410
N34	1.666670	1.333330	1.329470
H35	1.571100	1.525140	0.862340
Н36	1.571950	1.480070	1.217360
H37	1.616820	1.462360	1.420630
H38	1.574980	1.365040	1.007700
H39	1.601550	1.321490	1.035010

Table S2. Fractional atomic coordinates for the unit cell of Tfpa-Mth COF with staggered packing.

Tfpa-Mth COF with staggered packing			
Space group: P63 a = 39.29 Å, $b = 39.29$ Å, $c = 9.318$ Å $\alpha = \beta = 90^{\circ}, \gamma = 120^{\circ}$			
Atom	x/a	y/b	z/c
C1	1.914110	1.241840	0.391790
C2	1.936190	1.286000	0.355420
C3	1.924020	1.292920	0.205040
C4	1.980810	1.302200	0.365060
C5	1.941180	1.336520	0.169280

C6	1.793040	1.104280	0.429790
C7	1.779900	1.130810	0.394670
C8	1.790950	1.198570	0.355620
С9	1.806230	1.171540	0.386770
O10	1.809490	1.226810	0.276850
N11	1.756700	1.192590	0.416960
N12	1.743670	1.219680	0.395480
C13	1.712500	1.215770	0.459050
O14	1.767460	1.063190	0.440620
H15	1.923920	1.237530	0.498840
H16	1.921100	1.225810	0.308820
H17	1.928020	1.301390	0.437030
H18	1.891450	1.278910	0.199770
H19	1.933120	1.278880	0.121430
H20	1.990690	1.289310	0.279730
H21	1.988600	1.295070	0.470980
H22	1.997160	1.334730	0.354720
H23	1.973510	1.351100	0.153940
H24	1.934400	1.351650	0.255940
H25	1.928030	1.339380	0.067660
C26	1.677250	1.302960	0.422010
C27	1.720240	1.277900	0.349610
C28	1.708840	1.306370	0.339800
C29	1.656900	1.270200	0.512530
C30	1.668180	1.241680	0.521950
C31	1.700130	1.245420	0.441730
H32	1.749160	1.120130	0.372580
H33	1.741290	1.168940	0.487240
H34	1.695820	1.190990	0.530170
H35	1.744950	1.281510	0.286120
H36	1.724790	1.331260	0.268770
H37	1.632740	1.267110	0.578140
H38	1.652310	1.216960	0.593890
C39	1.728740	1.046430	0.381310
C40	1.707700	1.001230	0.390700
C41	1.730330	0.985060	0.304740
C42	1.665080	0.983610	0.337480
C43	1.714190	0.941020	0.328320
C44	1.846780	1.186350	0.409220
C45	1.859730	1.159920	0.447750
C46	1.848370	1.092850	0.501270
C47	1.833250	1.119380	0.460220
O48	1.835300	1.060910	0.442590

N49	1.877110	1.103980	0.603200
N50	1.893600	1.080180	0.632430
C51	1.922130	1.090530	0.723340
O52	1.872610	1.227330	0.395490
H53	1.711510	1.056830	0.443720
H54	1.730430	1.055360	0.266920
H55	1.706950	0.993250	0.505620
H56	1.761680	1.000550	0.338680
H57	1.729650	0.990770	0.188290
H58	1.664420	0.989030	0.220770
H59	1.649960	0.996990	0.395770
H60	1.648120	0.951450	0.357740
H61	1.684580	0.923440	0.279460
H62	1.712550	0.934300	0.444760
H63	1.734060	0.932180	0.276350
C64	1.978800	1.021540	0.770190
C65	1.924320	1.028590	0.680530
C66	1.943540	1.006900	0.692100
C67	1.993850	1.058270	0.838470
C68	1.974880	1.080250	0.825430
C69	1.940250	1.065820	0.744760
H70	1.890590	1.170520	0.467150
H71	1.887140	1.130480	0.658670
H72	1.934070	1.118440	0.779210
H73	1.897440	1.016570	0.618530
H74	1.931240	0.979000	0.636630
H75	2.020960	1.070420	0.898890
H76	1.987740	1.108950	0.875560
N77	1.666670	1.333340	0.417050
N78	2.000000	1.000000	0.775220