Supporting Information

Amino Group Induced Structural Diversity and Near-Infrared Emission of Yttrium-Tetracarboxylate Frameworks

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* To whom correspondence should be addressed: liuxiaoyuan1989@szpt.edu.cn jingli@rutgers.edu Y(NO₃)₃·6H₂O was purchased from Shanghai Aladdin Biochemical Technology Co., Ltd. Dimethyl 2'-amino-5'-bromo-[1,1':3',1"-terphenyl]-4,4"-dicarboxylate and dimethyl 5'-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-[1,1':3',1"-terphenyl]-4,4"-dicarboxylate were purchased from Jilin Chinese Academy of Science-Yanshen Technology Co., Ltd. 4,9-5',5""-(5,6-dimethylbenzo[c][1,2,5]thiadiazoledibromonaphtho[2,3-c][1,2,5]selenadiazole, 5'.5""-4,7-diyl)bis([1,1':3',1"-terphenyl]-4,4"-dicarboxylic acid) (H₄DTTC), (benzo[c][1,2,5]thiadiazole-4,7-diyl)bis(([1,1':3',1"-terphenyl]-4,4"-dicarboxylic acid)) 5',5'"'-(benzo[c][1,2,5]selenadiazole-4,7-diyl)bis(([1,1':3',1"-terphenyl]-4,4"- $(H_4BTTC),$ 5',5""-(naphtho[2,3-c][1,2,5]thiadiazole-4,9dicarboxylic acid)) (H_4BSTC), divl)bis(([1,1':3',1"-terphenyl]-4,4"-dicarboxylic acid)) (H₄NTTC), 5',5""'-(naphtho[2,3c][1,2,5]selenadiazole-4,9-diyl)bis(([1,1':3',1"-terphenyl]-4,4"-dicarboxylic acid)) (H₄NSTC) were synthesized according to our previous works.¹⁻² All the other chemicals were obtained from the chemical supplies and used without further purification.

Characterization

Nuclear magnetic resonance (NMR) data was collected using 400 MHz JEOL JNM-ECZ400S. Powder X-ray diffraction (PXRD) patterns were recorded using Bruker D8 Advance X-ray diffractometer with Cu K α radiation. Single crystal X-ray diffraction data were collected at 250 K on a Bruker D8 Venture diffractometer with Cu K α radiation or at 173 K on a 'Bruker D8 VENTURE Metaljet PHOTON II ' diffractometer equipped with gallium micro-focus metaljet X-ray sources ($\lambda = 1.34139$ Å). The solid-state photoluminescent spectra were measured on FLS1000 spectrofluorometer (Edinburgh Instruments) using the powder materials. The solid-state UV-vis spectra were recorded on Shimadzu UV-3600 spectrophotometer using the powder materials. The photoluminescent quantum yield was measured using C9920-03 absolute quantum yield measurement system (Hamamatsu Photonics) with a 150 W xenon monochromatic light source and 3.3 inch integrating sphere using sodium salicylate and YAG:Ce as the references. The TGA data was collected using TGA 550 (TA Instruments) analyzer and the samples were heated from room temperature to 600°C at a ramp rate of 10°C / min. Elementary analyses was recorded on Elementar Vario EL cube. The scanning electron microscopy-energy dispersive X-ray spectroscopy (SEM-EDS) was conducted on TESCAN MIRA LMS.

Density functional theory calculations

Structures of H₄BTTC, H₄ABTTC, H₄BTATC and H₄NSATC were optimized and characterized by frequency calculations to be energy minima (zero imaginary frequencies) at the B3LYP³/6-31g(d,p) level of density functional theory (DFT). The corresponding HOMO-LUMO energies were obtained from the output files. All calculations were performed with Gaussian 09.⁴

Organic synthesis

Synthesis of dimethyl 5'-(7-bromobenzo[c][1,2,5]thiadiazol-4-yl)-[1,1':3',1''-terphenyl]-4,4''-dicarboxylate



5'-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-[1,1':3',1"-terphenyl]-4,4"-dicarboxylate (5.0 mmol, 2.36 g), 4,7-dibromobenzo[c][1,2,5]thiadiazole (10.0 mmol, 2.93 g), PdCl₂ (0.4 mmol. 70.0 mg), PPh₃ (0.8 mmol, 0.21 g) and K2CO3 (16.0 mmol, 2.20 g) were added in a solution

containing 120 mL dioxane and 30 mL water. The mixture solution was degassed four times. Then the mixture solution was heated to reflux at 105 °C for 4 hours under nitrogen atmosphere. After cooling to room temperature, the solvent was removed under reduced pressure. The product dimethyl 5'-(7-bromobenzo[c][1,2,5]thiadiazol-4-yl)-[1,1':3',1"-terphenyl]-4,4"-dicarboxylate was obtained after purifying by silica gel column chromatography as a yellow solid (2.03 g, yield: 72.8%). ¹H NMR (400 MHz, CDCl₃) δ ppm 8.17 (2H), 8.15 (4H), 7.97 (1H), 7.93 (1H), 7.79 (4H), 7.71 (1H), 3.95 (s, 6H).



Synthesis of dimethyl 2'-amino-5'-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-[1,1':3',1''-terphenyl]-4,4''-dicarboxylate

Dimethyl 2'-amino-5'-bromo-[1,1':3',1"-terphenyl]-4,4"-dicarboxylate (5.0 mmol, 2.20 g), bis(pinacolato)diboron (6.0 mmol, 1.52 g), potassium acetate (14.2 mmol, 1.40 g,) and [1,1'-Bis(diphenylphosphino)ferrocene]dichloropalladium (0.07 mmol, 50.0 mg) were added into a 250 mL round-bottle flask containing 100 mL dioxane. The mixture was stirred at 110°C for 5 hours. After cooling down to room temperature, the reaction solution was filtered and the filtrate was removed under reduced pressure. The crude product was directly used for next step without further purification. ¹H NMR (400 MHz, CDCl₃) δ ppm 8.10 (4H), 7.59 (4H), 7.57 (2H), 3.94 (6H), 1.30 (12H).

Synthesis of dimethyl 2'-amino-5'-(7-(4,4''-bis(methoxycarbonyl)-[1,1':3',1''-terphenyl]-5'-yl)benzo[c][1,2,5]thiadiazol-4-yl)-[1,1':3',1''-terphenyl]-4,4''-dicarboxylate



5'-(7-bromobenzo[c][1,2,5]thiadiazol-4-yl)-[1,1':3',1"-terphenyl]-4,4"-dicarboxylate (2.0)mmol, 1.12 g), dimethyl 2'-amino-5'-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-[1,1':3',1"terphenyl]-4,4"-dicarboxylate (2.5 mmol, 1.22 g), PdCl₂ (0.2 mmol. 35.0 mg), PPh₃ (0.2 mmol, 0.11 g) and K2CO3 (8.0 mmol, 1.10 g) were added in a solution containing 80 mL dioxane and 20 mL water. The mixture solution was degassed four times. Then the mixture solution was heated to reflux at 105 °C for 5 hours under nitrogen atmosphere. During the reaction, the solid product was gradually generated. After cooling to room temperature, the crude 2'-amino-5'-(7-(4,4"-bis(methoxycarbonyl)-[1,1':3',1"-terphenyl]-5'product yl)benzo[c][1,2,5]thiadiazol-4-yl)-[1,1':3',1"-terphenyl]-4,4"-dicarboxylate filtered, was washed using water and dried as an orange solid, which was directly used for next step without further purification (1.59 g, yield: 94.8%).

Synthesisof2'-amino-5'-(7-(4,4''-dicarboxy-[1,1':3',1''-terphenyl]-5'-yl)benzo[c][1,2,5]thiadiazol-4-yl)-[1,1':3',1''-terphenyl]-4,4''-dicarboxylicacid(H₄ABTTC)



2'-amino-5'-(7-(4,4"-bis(methoxycarbonyl)-[1,1':3',1"-terphenyl]-5'-

yl)benzo[c][1,2,5]thiadiazol-4-yl)-[1,1':3',1"-terphenyl]-4,4"-dicarboxylate (1.5 mmol, 1.26 g) was added to a mixture solution containing 50 mL THF, 25 mL CH₃OH and 50 mL water with 4.0 g NaOH. The mixture solution was heated overnight at 85 °C. After cooling to room temperature, the mixture was filtered, and then the organic solvent was removed under reduced pressure. The filtrate was neutralized using 2M HCl to obtain the precipitate, which was filtered to offer the final product H₄ABTTC as a red orange solid (1.11 g, yield: 94.6%). ¹H NMR (400 MHz, DMSO-*d*₆) δ ppm 12.95 (4H), 8.33 (2H), 8.14 (1H), 8.08 (1H), 8.05 (8H), 8.00 (5H), 7.85 (2H), 7.71 (4H).



Synthesis of 5',5''''-(benzo[c][1,2,5]thiadiazole-4,7-diyl)bis(2'-amino-[1,1':3',1''terphenyl]-4,4''-dicarboxylic acid) (H₄BTATC)

Dimethyl 2'-amino-5'-bromo-[1,1':3',1"-terphenyl]-4,4"-dicarboxylate (4.0 mmol, 1.76 g), 4,7-

bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzo[c][1,2,5]thiadiazole (2.0 mmol, 0.78 g), PdCl₂ (0.2 mmol, 35.0 mg), PPh₃ (0.4 mmol, 0.11 g) and K₂CO₃ (8.0 mmol, 1.10 g) were added into a flask containing 80 mL 1,4-dioxane and 20 mL H₂O. After degassed four times, the mixture solution was heated and refluxed under nitrogen for 16 hours. After cooling down to room temperature, the solvent was removed under reduced pressure and 100 mL water was added. The mixture was filtered and the filtrate was neutralized using 2M HCl to obtain the precipitate, which was filtered to offer the final product H₄BTATC as a brown solid (1.56 g, 97.4%). ¹H NMR (400 MHz, DMSO- d_6) δ ppm 12.99 (4H), 8.04 (8H), 7.89 (2H), 7.79 (4H),7.68 (8H) ppm.



Synthesis of tetramethyl 5',5''''-(naphtho[2,3-c][1,2,5]selenadiazole-4,9-diyl)bis(2'amino-[1,1':3',1''-terphenyl]-4,4''-dicarboxylate)

Dimethyl 2'-amino-5'-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-[1,1':3',1"-terphenyl]-4,4"-dicarboxylate (5.0 mmol, 2.44 g), 4,9-dibromonaphtho[2,3-c][1,2,5]selenadiazole (2.0 mmol, 0.78 g), PdCl₂ (0.2 mmol, 35.0 mg), PPh₃ (0.4 mmol, 0.11 g) and K_2CO_3 (8.0 mmol, 1.10 g) were added in a solution containing 80 mL dioxane and 20 mL water. The mixture solution was degassed four times. Then the reaction mixture was heated to reflux at 105 °C for 24 h under nitrogen atmosphere. After cooling to room temperature, ID water was added and the crude product was filtered, washed using water and dried. Tetramethyl 5',5""-(naphtho[2,3-c][1,2,5]selenadiazole-4,9-diyl)bis(2'-amino-[1,1':3',1"-terphenyl]-4,4"-

dicarboxylate) was obtained as a dark red solid (1.78 g, 93.5%) and directly used for next step without further purification. ¹H NMR (400 MHz, DMSO- d_6) δ ppm 8.03 (8H), 7.95 (2H), 7.72 (8H), 7.29 (6H), 3.83 (12H).



Synthesis of 5',5''''-(naphtho[2,3-c][1,2,5]selenadiazole-4,9-diyl)bis(2'-amino-[1,1':3',1''terphenyl]-4,4''-dicarboxylic acid) (H₄NSATC)

Tetramethyl 5',5""-(naphtho[2,3-c][1,2,5]selenadiazole-4,9-diyl)bis(2'-amino-[1,1':3',1"terphenyl]-4,4"-dicarboxylate) (1.5 mmol, 1.43 g) was added to a mixture solution of 50 mL THF, 25 mL CH₃OH and 50 mL water with 4.0 g NaOH. The mixture was heated to reflux at 85 °C overnight. After cooling to room temperature, the reaction solution was filtered and the organic solvent was removed under reduced pressure. Then the aqueous was neutralized using 2M HCl to obtain the precipitate, which was filtered to offer the final product compound H₄NSATC as a blue-purple solid (1.24 g, 92.1%). ¹H NMR (400 MHz, DMSO- d_6) δ ppm 12.95 (4H), 8.01 (8H), 7.97 (1H), 7.68 (8H), 7.29 (3H), 7.21 (1H), 6.95 (3H).

Synthesis of HIAM-3900

Y(NO₃)₃·6H₂O (0.034 mmol, 13.0 mg), H₄DTTC (0.011 mmol, 8.50 mg), 2-fluorobenzoic

acid (150 mg) and 2.50 mL DMF were added in a 5 mL via. The mixture was heated in a 120 °C oven for 1 days. After cooling down to room temperature, the crystals were washed with DMF for several times until no fluorescent signal was detected from the supernatant. The colorless crystals of HIAM-3900 were collected by filtration, washed with DMF and hexane, and then dried in air with yield of 88.6%. Elemental analysis for HIAM-3900: Anal. Calcd (%) (according to the single crystal data of Y-**ftw**-MOF-2⁵ without dimethylammonium cations and solvent): 54.60; H, 3.66; N, 2.65%. Found: C, 40.08; H, 4.21; N, 2.35%.

Synthesis of HIAM-3901

 $Y(NO_3)_3 \cdot 6H_2O$ (0.034 mmol, 13.0 mg), H_4BTTC (0.011 mmol, 8.45 mg), 2-fluorobenzoic acid (250 mg) and 3.00 mL DMF were added in a 5 mL via. The mixture was heated in a 120 °C oven for 1 days. After cooling down to room temperature, the crystals were washed with DMF for several times until no fluorescent signal was detected from the supernatant. The light yellow crystals of HIAM-3901 were collected by filtration, washed with DMF and hexane, and then dried in air with yield of 85.2%. Elemental analysis for HIAM-3901: Anal. Calcd (%) (according to the single crystal data of Y-**ftw**-MOF-2⁵ without dimethylammonium cations and solvent): C, 53.73; H, 3.37; N, 2.72%. Found: C, 45.37; H, 3.23; N, 2.52%.

Synthesis of HIAM-3902

 $Y(NO_3)_3 \cdot 6H_2O$ (0.034 mmol, 13.0 mg), H_4BSTC (0.011 mmol, 9.00 mg), 2-fluorobenzoic acid (200 mg) and 2.50 mL DMF were added in a 5 mL via. The mixture was heated in a 120 °C oven for 1 days. After cooling down to room temperature, the crystals were washed with DMF for several times until no fluorescent signal was detected from the supernatant. The yellow crystals of HIAM-3902 were collected by filtration, washed with DMF and hexane, and then dried in air with yield of 81.9%. Elemental analysis for HIAM-3902: Anal. Calcd (%) (according to the single crystal data of Y-**ftw**-MOF-2⁵ without dimethylammonium cations and solvent): C, 51.33; H, 3.22; N, 2.60%. Found: C, 49.14; H,3.16; N, 2.71%.

Synthesis of HIAM-3903

 $Y(NO_3)_3 \cdot 6H_2O$ (0.034 mmol, 13.0 mg), H_4NTTC (0.011 mmol, 9.00 mg), 2-fluorobenzoic acid (200 mg) and 2.50 mL DMF were added in a 5 mL via. The mixture was heated in a 120 °C oven for 1 days. After cooling down to room temperature, the crystals were washed with DMF for several times until no fluorescent signal was detected from the supernatant. The orange crystals of HIAM-3903 were collected by filtration, washed with DMF and hexane, and then dried in air with yield of 86.6%. Elemental analysis for HIAM-3903: Anal. Calcd (%) (according to the single crystal data of Y-**ftw**-MOF-2⁵ without dimethylammonium cations and solvent): C, 55.69; H, 3.40; N, 2.60%. Found: C, 44.40; H, 3.58; N, 2.78%.

Synthesis of HIAM-3904

 $Y(NO_3)_3 \cdot 6H_2O$ (0.034 mmol, 13.0 mg), H_4NSTC (0.011 mmol, 9.52 mg), 2-fluorobenzoic acid (250 mg) and 2.50 mL DMF were added in a 5 mL via. The mixture was heated in a 120 °C oven for 1 days. After cooling down to room temperature, the crystals were washed with DMF for several times until no fluorescent signal was detected from the supernatant. The red crystals of HIAM-3904 were collected by filtration, washed with DMF and hexane, and then dried in air with yield of 82.2%. Elemental analysis for HIAM-3904: Anal. Calcd (%) (according to the single crystal data of Y-**ftw**-MOF-2⁵ without dimethylammonium cations and solvent): C, 53.32; H, 3.26; N, 2.49%. Found: C, 43.75; H, 3.61; N, 3.14%.

Synthesis of HIAM-3905

 $Y(NO_3)_3 \cdot 6H_2O$ (0.034 mmol, 13.0 mg), H_4ABTTC (0.011 mmol, 8.60 mg), 2-fluorobenzoic acid (300 mg) and 2.50 mL DMF were added in a 5 mL via. The mixture was heated in a 120 °C oven for 1 days. After cooling down to room temperature, the crystals were washed with DMF for several times until no fluorescent signal was detected from the supernatant. The orange crystals of HIAM-3905 were collected by filtration, washed with DMF and hexane, and then dried in air with yield of 89.6%. Elemental analysis for HIAM-3905: Anal. Calcd (%) (from single crystal data): C, 46.82; H, 1.85; N, 3.45%. Found: C, 43.61; H, 3.06; N, 4.40%.

Synthesis of HIAM-3906

 $Y(NO_3)_3 \cdot 6H_2O$ (0.034 mmol, 13.0 mg), H_4BTATC (0.011 mmol, 8.78 mg), 2-fluorobenzoic acid (250 mg) and 2.50 mL DMF were added in a 5 mL via. The mixture was heated in a 120 °C oven for 1 days. After cooling down to room temperature, the crystals were washed with DMF for several times until no fluorescent signal was detected from the supernatant. The red crystals of HIAM-3906 were collected by filtration, washed with DMF and hexane, and then dried in air with yield of 90.1%. Elemental analysis for HIAM-3906: Anal. Calcd (%) (from single crystal data): C, 50.75; H, 2.22; N, 5.10%. Found: C, 38.13; H, 3.83; N, 4.41%.

Synthesis of HIAM-3907

Y(NO₃)₃·6H₂O (0.034 mmol, 13.0 mg), H₄NSATC (0.011 mmol, 9.86 mg), 2-fluorobenzoic acid (200 mg) and 2.50 mL DMF were added in a 5 mL via. The mixture was heated in a 120 °C oven for 1 days. After cooling down to room temperature, the crystals were washed with DMF for several times until no fluorescent signal was detected from the supernatant. The dark red crystals of HIAM-3907 were collected by filtration, washed with DMF and hexane, and then dried in air with yield of 79.7%. Elemental analysis for HIAM-3907: Anal. Calcd (%)

(according to the single crystal of HIAM-3006): C, 52.72; H, 2.30; N, 4.88%. Found: C, 41.75; H, 3.67; N, 4.32%.

Single-crystal X-ray diffraction analyses

Single crystal of HIAM-3905 was mounted on MicroMesh (MiTeGen) with paraton oil. The data were collected on a 'Bruker D8 VENTURE Metaljet PHOTON II ' diffractometer equipped with gallium micro-focus metaljet X-ray sources ($\lambda = 1.34139$ Å). The crystals kept at the 173 K during data collection. Using Olex26, the structures were solved with the ShelXT⁷ structure solution program using Intrinsic Phasing and refined with the ShelXL⁸ refinement package using Least Squares minimization. In the structure HIAM-3905, the benzo[c][1,2,5]thiadiazole group and amino group of the HIAM-3905 ligands are found to be disordered over two sets of sites with occupancy of each part is 0.5. Furtherly in HIAM-3905, six Y^{3+} ions form an octahedron with the 8 faces each capped by a μ_3 -F. Eight of the edges of the octahedron are bridged by HIAM-3905 ligands via bidentate carboxylate groups with the remaining coordination sites of Y^{3+} are completed by formate ligands and H₂O molecules. The formate groups are found to be disordered over two parts (with occupancy of part 1: part 2 = 0.547:0.453). In the structure of part 1, formate ligands act as bridging ligands in a bismonodentate syn-syn mode, while in the structure of part 2, formate ligands act as terminal ligands in chelate mode. Formate groups were refined using geometry restrains (DFIX), and restraints were also used to refine formate groups and the benzo[c][1,2,5]thiadiazole group (SIMU, DELU, ISOR, EADP). The hydrogen atoms on the aromatic rings were located at geometrically calculated positions and refined by riding. However, the hydrogen atoms for the

coordinated molecules cannot be found from the residual electron density peaks and the attempt of theoretical addition was not done. The free solvent molecules are highly disordered in MOFs, and attempts to locate and refine the solvent peaks were unsuccessful. The diffused electron densities resulting from these solvent molecules were removed using the Solvent Mask routine of Olex2, structures were then refined again using the data generated. The refinement results are summarized in Table S1.

Single crystals of HIAM-3906 were mounted on MicroMesh (MiTeGen) with paraton oil. The data were collected on a 'Bruker D8 VENTURE' diffractometer equipped with copper micro-focus X-ray sources ($\lambda = 1.5406$ Å). The crystals kept at the 250 K during data collection. Using Olex2⁶, the structures were solved with the ShelXT⁷ structure solution program using Intrinsic Phasing and refined with the ShelXL⁸ refinement package using Least Squares minimization. In the structure HIAM-3906, the benzo[c][1,2,5]thiadiazole group of the H₄BTATC ligands are all disordered. Furtherly in HIAM-3906, six Y³⁺ ions form an octahedron with the 8 faces each capped by a μ_3 -F. Ten of the edges of the octahedron are bridged by BTATC ligands via bidentate carboxylate groups with the remaining coordination sites of Y³⁺ are completed by formate groups or H₂O molecules (with occupation factor of 0.5:0.5). Disordered atoms were refined using geometry restrains (SADI, DFIX, FLAT), and restraints were also used to refine anisotropic displacement parameters of all non-hydrogen atoms (SIMU and DELU). The hydrogen atoms on the aromatic rings were located at geometrically calculated positions and refined by riding. However, the hydrogen atoms for the coordinated molecules cannot be found from the residual electron density peaks and the attempt of theoretical addition was not done. The free solvent molecules are highly disordered

in MOFs, and attempts to locate and refine the solvent peaks were unsuccessful. The diffused electron densities resulting from these solvent molecules were removed using the SQUEEZE routine of PLATON⁹; structures were then refined again using the data generated. The refinement results are summarized in Table S2.

Crystallographic data for all of the crystal structures in CIF format have been deposited in the Cambridge Crystallographic Data Centre (CCDC) under deposition number CCDC-2165296 (HIAM-3905) and CCDC-2151211 (HIAM-3906). The data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, U.K.)



Figure S1. The normalized emission spectrum of H_4ABTTC and H_4BTATC in DMF under 365 nm excitation.



Figure S2. Single crystal structure of HIAM-3905 viewed along *a* axis (left) and *b* axis (right).



Figure S3. Single crystal structure of HIAM-3906 viewed along *a* axis (left) and *b* axis (right).



Figure S4. Conformations of the tetratopic ligands in HIAM-3901 (the single crystal structure was adapted from the reported work⁵ and the thiadiazole ring was omitted for clarity).



Figure S5. EDS data of HIAM-3905.



Figure S6. EDS data of HIAM-3906.

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Figure S7. PXRD of as-synthesized HIAM-3907 and after immersed in water for 12 hours.



Figure S8. The TGA curve of as-synthesized HIAM-3900, HIAM-3901, HIAM-3902, HIAM-3903 and HIAM-3904.



Figure S9. The TGA curve of as-synthesized HIAM-3905, HIAM-3906 and HIAM-3907.

Table S1. Crystal data and structure refinement parameters for HIAM-3905.		
CCDC No.	2165296	
Empirical formula	C47.48 H22.52F4 N3 O12.97 S Y3	
Formula weight	1217.37	
Temperature	173 K	
Wavelength	1.34139 Å	
Crystal system	orthorhombic	
Space group	Cmmm	
Unit cell dimensions	$a = 21.358(10) \text{ Å} \qquad \alpha = 90^{\circ}$	
	$b = 35.038(16) \text{ Å} \qquad \beta = 90^{\circ}$	
	$c = 20.494(9) \text{ Å} \qquad \gamma = 90^{\circ}$	
Volume	15337(12) Å ³	
Z	4	
Density (calculated)	0.527 Mg/m ³	
Absorption coefficient	1.230 mm ⁻¹	
F(000)	2405.0	
Crystal size	0.12 x 0.11 x 0.1 mm ³	
Theta range for data collection	4.216 to 107.812°	
Index ranges	-25<=h<=25, -42<=k<=38, -24<=l<=	24
Reflections collected	47876	
Independent reflections	7538[R(int) = 0.1519, R(sigma) = 0.0	819]
Data / restraints / parameters	7538/93/191	
Goodness-of-fit on F ²	0.922	
Final R indices [I>2sigma(I)]	R1 = 0.0853, wR2 = 0.2230	
R indices (all data)	R1 = 0.1227, wR2 = 0.2530	
Largest diff. peak and hole	$1.23 \text{ and } -0.62 \text{ e.}\text{Å}^{-3}$	

Table S2. Crystal data and structure refinement parameters for HIAM-3906.	
CCDC No.	2151211
Empirical formula	C232 H122F16 N20 O48 S5 Y12
Formula weight	5488.71
Temperature	250 К
Wavelength	1.54178 Å
Crystal system	orthorhombic
Space group	Cmmm
Unit cell dimensions	$a = 40.568(2) \text{ Å} \qquad \alpha = 90^{\circ}$
	$b = 41.959(2) \text{ Å} \qquad \beta = 90^{\circ}$
	$c = 19.6114(13) \text{ Å} \qquad \gamma = 90^{\circ}$
Volume	33382(3) Å ³
Z	2
Density (calculated)	0.546 Mg/m ³
Absorption coefficient	1.746 mm ⁻¹
F(000)	5460.0
Crystal size	0.130 x 0.070 x 0.070mm ³
Theta range for data collection	5.43 to 134.852°
Index ranges	-48<=h<=33, -49<=k<=49, -20<=l<=23
Reflections collected	70779
Independent reflections	15675[R(int) = 0.1039, R(sigma) = 0.0758]
Data / restraints / parameters	15675/595/522
Goodness-of-fit on F ²	0.950
Final R indices [I>2sigma(I)]	R1 = 0.0589, wR2 = 0.1711
R indices (all data)	R1 = 0.0743, wR2 = 0.1807
Largest diff. peak and hole	0.690 and -0.670 e.Å ⁻³

References

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