Enhancing Charge Mobilities in Selectively Fluorinated Oligophenyl Organic Semiconductors: A Design Approach Based on Experimental and Computational Perspective
– Supporting Information (SI) –

Buddhadev Maiti,[†,‡] Kunlun Wang,[†,‡] Srijana Bhandari,[†,‡] Scott D. Bunge,[†] Robert J. Twieg,[†] and Barry D. Dunietz[*,†]

Department of Chemistry and Biochemistry, Kent State University, Kent, Ohio 44242, USA

Received January 25, 2019; E-mail: bdunietz@kent.edu

[†]Department of Chemistry and Biochemistry, Kent State University, Kent, Ohio 44242, USA

[‡]Contributed equally to this work.

1 Experimental Data

1.1 Reagents

All the reagents were obtained from commercial sources and used without further purification. Commercial-grade solvents were used except in the case of tetrahydrofuran which was dried over sodium / benzophenone prior to use. Palladium tetrakistriphenylphosphine was prepared according to the literature[1] from palladium dichloride, which was purchased from Pressure Chemical (Pittsburgh, PA). $Pd(dppf)Cl_2$ was purchased from Sigma-Aldrich. n-Butyllithium and ether were purchased from Acros. The fluorophenylboronic acids were synthesized or purchased from Combi-Blocks (San Diego, CA). The molecules prepared here were purified either by column chromatography using silica gel (60 - 120 mesh) or by recrystallization from analytical grade solvents. Differential scanning calorimetry (DSC) analysis was run on a 2920 modulated DSC from TA instruments (TA Instruments Inc., New Castle, DE, USA). Experimental data was analyzed and exported by using the Thermal Advantage software (Version 1.1A, TA Instruments Inc., New Castle, DE, USA).

2,3-Difluorophenylboronic acid

Into a 250 ml round bottom two-neck flask under a nitrogen atmosphere was added anhydrous THF (80 ml), 1,2-difluorobenzene (3.4 g, 30.0 mmol) and the mixture was cooled to -78°C. Next, n-butyllithium (12 ml, 30.0 mmol, 1.0 equiv., 2.5 M in hexanes) was added to this solution over a period of 10 minutes and stirred at the same temperature for 1 hour. Triisopropyl borate (11.4 g, 60.0 mmol, 2.0 equiv.) was dissolved in 10 ml of dry THF and added to the reaction mixture which was then allowed to warm up to room temperature slowly and stirred overnight. The reaction mixture was quenched with 10% HCl (80 ml) and extracted with diethyl ether (400 ml). After washing with water (300 ml) and brine (100 ml), the organic layers were combined and dried with $MgSO_4$, and the solvent removed by rotary evaporation. The residue was recrystallized from hexanes to afford 4.4 g (93% yield) of a light yellow solid (very polar). ^{1}H NMR (400 MHz, DMSO-d6) δ (ppm): 7.57 (m, ^{1}H), 7.31 -7.24 (m, 1H), 7.14 (m, 1H), 5.27 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -135.91, -139.29. The data was consistent with the reference.[2]

2,3-Difluoroiodobenzene

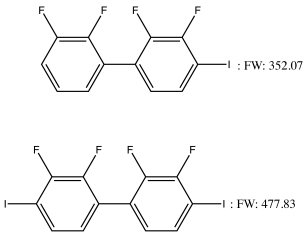
Into a 250 ml round bottom two-neck flask under a nitrogen atmosphere was added anhydrous THF (80 ml), 1,2-difluorobenzene (3.4 g, 30.0 mmol) and the mixture was cooled to -78°C. Next, n-butyllithium (12 ml, 30.0 mmol, 1.0 equiv., 2.5 M in hexanes) was added to this solution over a period of 10 minutes and stirred at the same temperature for 1 hour. Iodine (15.2 g, 60.0 mmol, 2.0 equiv.) was dissolved in 20 ml of dry THF and added to the reaction mixture which was then allowed to warm up to room temperature slowly and stirred overnight. The reaction mixture was quenched with 10% HCl (80 ml) and extracted with diethyl ether (400 ml). After washing with water (300 ml), saturated sodium thiosulfate solution (30 ml) and brine (100 ml), the organic layers were combined and dried with $MgSO_4$, and the solvent removed by rotary evaporation to afford 6.6 g (92 %) of a yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.48 (m, 1H),7.14 (m, 1H), 6.85 (m, 1H). The data was consistent with the reference.[3]

2,3,2',3'-Tetrafluorobiphenyl (**1**)

In a 200 ml round bottom flask fitted with a magnetic stirbar was dissolved 2,3-difluoroiodobenzene (4.8 g, 20.0 mmol) in a mixture of H_2O (20 ml) and 1,4-dioxane (50 ml) to give a light yellow solution. $Pd(PPh_3)_4$ (230 mg, 1 mol%) and 2,3-difluorophenylboronic acid (4.72 g, 1.5 equiv., 15.0 mmol) were added to the solution and the mixture was stirred at room temperature for 5 minutes. Next, potassium carbonate (8.3 g, 3.0 equiv.) was added and the mixture was stirred and refluxed for 48 hours until TLC analysis indicated the completion of the reaction. The mixture was cooled and poured into a 250 ml separatory funnel and the organic layer was separated. The aqueous layer was extracted with ethyl acetate (60 ml) twice and the combined organic layers were dried with $MgSO_4$. Column chromatography on silica gel (eluted with hexanes) was used to purify the desired product (white crystals after evaporation, 2.6 g, 60%). Melting point: 82-83°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.24-7.20 (m, 2H), 7.17-7.14 (m, 2H), 7.13-7.11 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 152.5-150.0 (d, J = 241.8, 2C), 149.7-147.0 (d, J = 247.1, 2C), 133.4, 126.1, 124.1, 117.4 (d, J = 17.1, 2C); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -137.42 (m, 2F), -139.38 (m, 2F). GC/MS: 226.13 found, 226.17 calc.

4-Iodo-2,3,2',3'-tetrafluorobiphenyl (**2**) and 4,4'-diiodo-2,3,2',3'-tetrafluorobiphenyl (**3**)

Into a 100 ml round bottom two-neck flask, 1,1',2,2'-tetrafluorobiphenyl (1.1 g, 5.0 mmol) and anhydrous THF (40 ml) was added under a nitrogen atmosphere and the mixture was cooled to -78°C. Next, n-butyllithium (2.0 ml, 5.0 mmol, 1.0 equiv., 2.5 M in hexanes) was added to this solution over a period of 5 minutes and stirred at the same temperature for 1 hour. Iodine (2.6 g, 10.0 mmol, 2.0 equiv.) was dissolved in 10 ml of dry THF and added to the mixture which was then allowed to warm up to room temperature slowly and stirred overnight. The reaction mixture was then quenched with water and extracted with diethyl ether (300 ml). After washing with water (300 ml), saturated sodium thiosulfate solution (30 ml) and brine (50 ml), the organic layers were combined and dried with $MgSO_4$, and the solvent removed by rotary evaporation to afford a yellow solid (1.3 g, 37%, of **2** based on 1,1',2, 2'-tetrafluorobiphenyl) after storage in a freezer. GC/MS: 352.07, 477.83 (1:2 ratio of monoiodination and diiodination adduct by NMR)



SI Figure 1. The structure of 4-Iodo-2,3,2',3'-tetrafluorobiphenyl (**2**) and 4,4'-diiodo-2,3,2',3'-tetrafluorobiphenyl (**3**).

2,3,2',3',2",3"-Hexafluoro-[1,1';4',1"]terphenyl (**4**)

In a 200 ml round bottom flask fitted with a magnetic stirbar was dissolved the 4-iodo-2,3,2',3'-tetrafluorobiphenyl (1.3 g, 2.8 mmol calc. by diiodide) in a mixture of H_2O (8 ml) and 1,4-dioxane (20 ml)to give a light yellow solution. $Pd(PPh_3)_4$ (33 mg, 1 mol%) and 2,3-difluorophenylboronic acid (4.72 g, 2.5 equiv., 2.2 mmol) were added and the mixture was stirred at room temperature for 5 minutes. Next, potassium carbonate (1.5 g, 4.0 equiv.) was added and the mixture was stirred and refluxed for 24 hours until TLC analysis indicated completion of the reaction. The mixture was cooled and poured into a 250 ml separatory funnel and the organic layer was separated. The aqueous layer was extracted with 60 ml ethyl acetate twice and the combined organic layers were dried with $MgSO_4$. Column chromatography on silica gel (eluted with hexanes) was used to purify the product (a white solid after evaporation, 280 mg, 32 %). Melting point: 170.8°C (sublimes). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.30-7.24 (m, 4H), 7.23-7.17 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 150.9 (dd, ^{1}J = 198.0 Hz, ^{2}J = 10.4, 2C), 148.1 (ddd, ^{1}J = 201.8 Hz, ^{2}J = 12.5, ^{3}J = 10.4, 4C), 126.1 (t, J = 1.4, 2C), 125.6 (dd, ^{1}J = 4.1 Hz, ^{2}J = 2.7, 4C), 124.2 (dd, ^{1}J = 5.6 Hz, ^{2}J = 3.8, 4C), 117.6 (d, J = 13.7, 2C); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -137.16 (m, 2F), -138.15 (m, 2F), -139.21 (m, 2F); GC/MS: 338.06 found, 338.25 calc.

4,4'-Diiodo-2,3,2',3'-tetrafluorobiphenyl (**3**)

A 250 ml round bottom two-neck flask was charged with 2,2',3,3'-tetrafluorobiphenyl (1.1 g, 5.0 mmol), anhydrous THF (30 ml) under a nitrogen atmosphere and the resulting mixture was cooled to -78°C. Next, n-butyllithium (5 ml, 12.5 mmol, 2.5 equiv., 2.5 M in hexanes) was injected over a period of 10 minutes and this mixture was stirred at -78°C for 2 hours. Iodine (5.1 g, 20.0 mmol, 2.0 equiv.) dissolved in 10 ml of dry THF was added to the reaction mixture, which was allowed to slowly warm up to room temperature with stirring overnight. The reaction mixture was then quenched with water (100 ml) and extracted with diethyl ether (300 ml). After washing with water (200 ml), saturated sodium thiosulfate solution (30 ml) and brine (100 ml), the organic layers were combined and dried with $MgSO_4$ and the solvent removed by rotary evaporation to afford 2.0 g of a yellow liquid. Column chromatography on silica gel (hexane as the eluent) was used to purify the product and a yellow liquid was collected eventually after evaporation (1.8 g, 75% yield of 3 based on 1,1',2, 2'-tetrafluorobiphenyl). GC/MS: 477.69, 351.85. The product mixture contained both monoadduct and diadduct (same Rf value) even though 2.5 equiv. of n-butyllithium was used.

2,3,2',3',2",3",2"',3"'-Octafluoro-[1,1';4',1";4",1"']quaterphenyl (**5**)

In a 200 ml round bottom flask fitted with a magnetic stirbar was dissolved 4,4'-diiodo-2,3,2',3'-tetrafluorobiphenyl (0.9 g, 2.0 mmol calc. by diiodide) in a mixture of H_2O (8 ml) and 1,4-dioxane (20 ml) to give a light yellow solution. $Pd(PPh_3)_4$ (27 mg, 1 mol%) and 2,3-difluorophenylboronic acid (1.2 g, 4.0 equiv., 8.0 mmol) were added and the mixture was stirred at room temperature for 5 minutes. Next, potassium carbonate (2.2 g, 4.0 equiv.) was added and the mixture was stirred and refluxed for 48 hours until TLC analysis indicated the disappearance of the starting material and the formation of one new molecule that didn't move in hexane. After cooling to room temperature, H_2O (100 ml) was added and the resulting white solids were vacuum filtered followed by a hot filtration and crystallization process with toluene (a white solid after evaporation, 240 mg, 27 %). Melting point: 247.0°C (sublimes). ^{1}H NMR (400 MHz, tetrachloroethane-d_2, 75°C) δ (ppm): 7.38-7.31 (m, 10H); ^{13}C NMR (100 MHz, tetrachloroethane-d_2, 75°C) δ (ppm): 152.3, 149.8, 147.2, 126.3, 125.9, 125.8, 124.9, 124.5, 124.3, 117.8; ^{19}F NMR (376 MHz, tetrachloroethane-d_2, 75°C) δ (ppm): -136.66 (m, 2F), 137.50 (s, 4F), 138.67 (s, 2F). GC/MS: 450.02 found 450.32 calc.

2,5-Difluorophenyl Bpin (**6**)

A mixture of 2,5-difluorobromobenzene (5.79 g, 30.0 mmol), potassium acetate (8.7 g, 45.0 mmol) in anhydrous DMF (80 ml) was stirred at room temperature under a nitrogen atmosphere for 15 minutes followed by the addition of bis(pinacolato)diboron (9.1 g, 36.0 mmol, 1.2 equiv.) and palladium tetrakis(triphenylphosphine) (230 mg, 0.2 mmol, 0.5% mol%). The mixture was then heated to 80°C and stirred overnight. TLC analysis indicated the disappearance of the 2,5-difluorobromobenzene. After cooling to room temperature, the remaining solids were filtered off. The filtrate was dried under vacuum, redissolved in ethyl acetate (200 ml) then washed with water (3x200 ml) and brine (100 ml). The organic layer was dried over magnesium sulfate and condensed to give light green oil which was purified by column chromatography to give light green crystals after storage in the freezer (6.2 g, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.38 (m, 1H), 7.08 (m, 1H), 6.97 (m, 1H), 1.36 (s, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.2, 161.7, 159.6, 157.2, 122.4, 122.3, 122.1, 119.9, 119.6, 116.6, 84.3, 24.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -109.41 (m, 1F), -120.57 (m, 1F).

2,5,2',5'-Tetrafluorobiphenyl (**7**)

In a 100 ml round bottom flask fitted with a magnetic stirbar 2,5-difluorobromobenzene (1.93 g, 10.0 mmol) was dissolved in a mixture of H_2O (8 ml) and 1,4-dioxane (20 ml) to give a colorless solution. $Pd(PPh_3)_4$ (115 mg, 1 mol) and 2,5-difluorophenyl Bpin (2.88 g, 1.2 equiv., 12.0 mmol) were added and the mixture was stirred at room temperature for 10 minutes. Next, potassium carbonate (5.5 g, 4.0 equiv.) was added and the mixture was stirred and refluxed for 24 hours until TLC analysis indicated the completion of the reaction. The mixture was cooled and poured into a 250 ml separatory funnel and the organic layer was separated. The aqueous layer was extracted with ethyl acetate (60 ml)twice and the combined organic layers were dried with $MgSO_4$. Column chromatography on silica gel (eluted with hexanes) was used to purify the desired product as white crystals after evaporation (1.5 g, 66%). GC/MS: found 226.03, calc. 226.17. Melting point: 78.1-78.8°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.17-7.05 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 159.6-156.8 (d, J = 268.3, 2C), 157.3-154.5 (d, J = 271.5, 2C), 123.7 (m, 1C), 117.8 (m, 1C), 116.6 (m, 1C); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -118.86 (m, 2F), -120.87 (m, 2F).

2,5,2',5',2",5"-Hexafluoro-[1,1';4',1"]terphenyl (**8**)

In a 100 ml round bottom flask fitted with a magnetic stirbar 2,5-difluoro-1,4-dibromobenzene (1.37 g, 5.0 mmol) was dissolved in a mixture of H_2O (8 ml) and 1,4-dioxane (20 ml) to give a colorless solution. $Pd(PPh_3)_4$ (115 mg, 1 mol%) and 2,5-difluorophenyl Bpin (2.88 g, 2.4 equiv., 12.0 mmol) were added and the mixture was stirred at room temperature for 10 minutes. Next, potassium carbonate (5.5 g, 4.0 equiv.) was added and the mixture was stirred and refluxed for 24 hours until TLC analysis indicated the completion of the reaction and the formation of two molecules (one quite polar). The mixture was cooled and poured into a 250 ml separatory funnel and the organic layer was separated. The aqueous layer was extracted with ethyl acetate (60 ml)twice and the combined organic layers were dried with $MgSO_4$. Column chromatography on silica gel (eluted with hexanes) was used to purify the desired product as white crystals after evaporation (0.3 g, 22 %). Melting point: 180-181°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.26-7.19 (m, 2H), 7.18-7.10 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 159.7-157.3 (d, J = 272.5, 2C), 157.3-154.5 (d, J = 274.5, 2C), 156.6-154.2 (d, J = 244.9, 2C), 123.5 (m, 2C), 118.4 (m, 1C), 117.9-117.0 (m, 2C), 116.8-116.7 (m, 1C); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -118.60 (m, 2F), -120.15 (m, 2F), -120.63 (m, 2F); GC/MS: 338.06 found, 338.25 calc.

4-Bromo-2,5,2',5'-tetrafluorobiphenyl (**9**)

A 200 ml round bottom flask fitted with a magnetic stirbar was charged with 1,4-dibromo-2,5-difluorobenzene (8.22 g, 30.0 mmol) and a mixture of H_2O (16 ml) and 1,4-dioxane (50 ml) to give a colorless solution. Next, $Pd(PPh_3)_4$ (165 mg, 0.5 mol%) and 2,5-difluorophenyl Bpin (8.64 g, 1.2 equiv., 36.0 mmol) were added and the mixture was stirred at room temperature for 10 minutes followed by the addition of potassium carbonate (12.4 g, 3.0 equiv.) This mixture was then stirred at 80°C for 24 hours until TLC analysis indicated the disappearance of 1,4-dibromo-2,5-difluorobenzene and the formation of two new molecules. The mixture was cooled, poured into a 250 ml separatory funnel and extracted with ethyl acetate (60 ml) twice and the combined organic layers were dried with $MgSO_4$. Column chromatography on silica gel (eluted with hexanes) was used to purify the desired product as white crystals after evaporation (3.4 g, 37% yield). Melting point: 77-78°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.19 (m, 1H), 7.17 (m, 1H), 7.14-7.08 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 159.6-157.2 (d, J = 238.1, 2C), 156.9-154.5 (d, J = 241.1, 2C), 121.0, 120.7, 118.4-116.5 (d, J = 190.8, 2C), 110.3 (m, 2C); ^{19}F NMR (376MHz, $CDCl_3$) δ (ppm): -112.12 (m, 1F), -118.64-119.01(m, 2F), 120.87 (m, 1F). GC/MS: 303.96/305.93 (twin peaks for bromine atom) found 304.06 calc.

2,5,2',5'-Tetrafluoro-biphenyl-4-Bpin (**10**)

A mixture of 4-bromo-2,2',5,5'-tetrafluorobiphenyl (912 mg, 3.0 mmol), potassium acetate (0.5 g, 3.0 mmol) in 1,4-dioxane (20 ml) was stirred at room temperature under a nitrogen atmosphere for 15 minutes. Bis(pinacolato)diboron (1.0 g, 4.0 mmol, 1.3 equiv.) and palladium tetrakis(triphenylphosphine) (56 mg, 0.05 mmol, 1.6 mol%) were then added and the resulting mixture was heated to 80°C and stirred overnight. TLC analysis indicated the formation of one new molecule but still some starting material iodide was left. The reaction was kept for another 12 hours at 100°C and TLC analysis indicated the disappearance of the starting material. After removing the solvent by rotary evaporation, the remaining solids were dissolved with hexanes and the filtrate was purified by a short column on silica gel to give the desired product as a light yellow solid after evaporation without further purification (950 mg, 90%) and melting point is 44-45°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.69-7.64 (m, 2H), 7.54 (m, 1H), 7.48-7.46 (m, 2H), 1.27 (s, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 159.6-157.2 (d, J = 239.8, 1C), 132.1(m, 1C), 128.5 (d, J = 12.1, 1C), 117.9 (m, 2C), 116.8-116.6 (m, 1C), 116.1, 115.9, 105.5 (d, J = 28.0, 2C), 84.4, 83.2, 24.8, 24.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -112.15 (m, 1F), -118.67-119.05 (m, 2F), 120.89 (m, 1F).

2,5,2',5',2",5",2"',5"'-Octafluoro-[1,1';4',1";4",1"']quaterphenyl (**11**)

In a 200 ml round bottom flask fitted with a magnetic stirbar, 4-bromo-2, 2',5,5'-tetrafluorobiphenyl (608 mg, 2.0 mmol) was dissolved in a mixture of H_2O (6 ml) and 1,4-dioxane (15 ml) to give a colorless solution. Next, $Pd(PPh_3)_4$ (56 mg, 1.0 mol%) and 2,2',5,5'-tetrafluorobiphenyl-4-Bpin (875 mg, 1.25 equiv., 2.5 mmol) were added and the mixture was stirred at room temperature for 10 minutes followed by the addition of potassium carbonate (1.1 g, 4.0 equiv.) This mixture was stirred and refluxed for 48 hours and a white precipitate was formed. TLC analysis (eluted with hexanes: ethyl acetate = 10:1) indicated the appearance of unreacted 4-bromo-2,2',5,5'-tetrafluorobiphenyl and the formation of one new fluorescent molecule that was slightly more polar. After cooling to the room temperature, water (200 ml) was added to the mixture and the resulting grey precipitate was vacuum filtered and washed with H_2O to give a grey crude product. The solids were then boiled with silica gel and K-10 clay in toluene and hot filtered by gravity. The filtrate was then concentrated and cooled to crystallize a white solid which was vacuum filtered. (190 mg, 42%) ^{1}H NMR (400 MHz, DMSO d6 at 65°C) δ (ppm): 7.37 (d, J = 4.0, 4H), 7.27-7.19 (m, 6H); ^{13}C NMR (100 MHz, DMSO d6 at 65°C) δ (ppm): 159.9, 156.3, 154.4, 141.3, 138.3, 134.5, 130.4, 124.7, 123.3, 122.2, 118.7, 118.0, 117.8, 117.2, 106.7; ^{19}F NMR (376 MHz, DMSO d6 at 65°C) δ (ppm):-117.89 (m, 2F), -119.19 (m, 4F), -119.82 (m, 2F), GC/MS: 450.10 found 450.32 calc. Melting point: 264-265°C.

2,6-Difluoroiodobenzene

To a solution of hydrochloric acid (60 ml) in H_2O (60 ml) was added 2,6-difluoroaniline (7.74 g, 60.0 mmol). The resulting suspension was cooled to 0°C and was added first a solution of $NaNO_2$ (8.28 g, 120 mmol) in H_2O (60 ml) and next a solution of KI (24.9 g, 150 mmol) in H_2O (60 ml), dropwise. The resulting mixture was stirred for 10 minutes then allowed to warm to room temperature and stirred overnight. The mixture was extracted with diethyl ether (150 ml) three times. The organic layers were combined and washed with H_2O, brine and dried with $MgSO_4$. TLC indicated only one new product with lower polarity than the starting material. The desired product was purified by chromatography column on silica gel eluted with hexanes to give a colorless oil after evaporation (10 g, 70%). GC/MS: 239.9 found, 239.9 calc. This is a known substance.[4]

3,5-Difluorophenyl Bpin (**12**)

A mixture of 3,5-difluorobromobenzene (5.79 g, 30.0 mmol), potassium acetate (8.7 g, 45.0 mmol) in anhydrous DMF (80 ml) was stirred at room temperature under a nitrogen atmosphere for 15 minutes followed by the addition of bis(pinacolato)diboron (9.1 g, 36.0 mmol, 1.2 equiv.) and palladium tetrakis(triphenylphosphine) (230 mg, 0.2 mmol, 0.5% mol%). The mixture was then heated to 80°C and stirred for 5 hours. TLC analysis indicated the disappearance of the starting material 3,5-difluorobromobenzene. After cooling to room temperature, the remaining solids were filtered off. The filtrate was condensed by rotary evaporation, dissolved in ethyl acetate (100 ml) then washed with water (3x200 ml) and brine (100 ml). The organic layers were dried over magnesium sulfate and condensed to give a light green oil which was purified by column chromatography to give light green crystals after evaporation (6.3 g, 88%). Melting point: 34-35°C (Ref. 36-38°C).[5]

2,6,3',5'-Tetrafluorobiphenyl (**13**)

In a 100 ml round bottom flask fitted with a magnetic stirbar 2,6-difluoroiodobenzene (2.4 g, 10.0 mmol) was dissolved in a mixture of H_2O (8 ml) and 1,4-dioxane (20 ml) to give a colorless solution. $Pd(dppf)Cl_2$ (75 mg, 1 mol%) and 2,3-difluorophenyl Bpin (2.88 g, 1.2 equiv., 12.0 mmol) were added and the mixture was stirred at room temperature for 10 minutes. Next, potassium carbonate (5.5 g, 4.0 equiv.) was added and the mixture was stirred and refluxed for 24 hours until TLC analysis indicated the completion of the reaction. The mixture was cooled and poured into a 250 ml separatory funnel and the organic layer was separated. The aqueous layer was extracted with ethyl acetate (60 ml) twice and the combined organic layers were dried with $MgSO_4$. Column chromatography on silica gel (eluted with hexanes) was used to purify the desired product as white crystals after evaporation (1.4 g, 64 %). Melting point: 89.1-89.6°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.31 (m, 2H), 7.00 (m, 2H), 6.86 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 163.9-161.0 (d, J = 292.1, 2C), 161.6-158.6 (d, J = 294.0, 2C), 132.1, 130.7, 113.4, 111.5, 109.9 (d, J = 7.0, 1C), 103.7 (t, J = 25.1, 2C); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -110.11 (m, 2F), -114.12 (m, 2F). GC/MS: 226.10 found, 226.17 calc.

4'-Iodo-2,6,3',5'-tetrafluorobiphenyl (**14**)

Into a 100 ml round bottom two-neck flask under a nitrogen atmosphere, 2,3',5',6-tetrafluorobiphenyl (1.1 g, 5.0 mmol), anhydrous THF (50 ml) was added and the mixture was cooled to -78°C. Next, n-butyllithium (3.0 ml, 7.5 mmol, 1.5 equiv., 2.5 M in hexanes) was added to this solution over a period of 5 minutes and stirred at the same temperature for 1.5 hours. Iodine (2.54 g, 10.0 mmol, 2.0 equiv.) was dissolved in 15 ml of dry THF and added. The resulting mixture was allowed to warm up to room temperature slowly and stirred overnight. This mixture was then quenched with water and extracted with diethyl ether (100 ml). After washing with water (200 ml), saturated sodium thiosulfate solution (20 ml), the organic layers were combined and dried with $MgSO_4$. The solvent was removed by rotary evaporation to afford the product as a yellow liquid (1.6 g, 91 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.37-7.30 (m, 1H), 7.03-6.98 (m, 3H), 6.89-6.85 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 163.8-161.4 (d, J = 246.2, 2C), 161.1- 158.6 (d, J = 249.7, 2C), 152.5, 132.1, 131.0, 130.5, 130.0-129.8 (d, J = 23.1, 2C), 113.6, 111.9 (m, 1C), 103.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -109.52 (m, 2F), -112.15 (m, 2F).

4-Bromo-2,6,3',5'-tetrafluorobiphenyl (**15**)

In a 100 ml round bottom flask fitted with a magnetic stirbar 4-bromo-2,6-difluoroiodobenzene (3.14 g, 10.0 mmol) was dissolved in a mixture of H_2O (8 ml) and 1,4-dioxane (20 ml) to give a colorless solution. $Pd(dppf)Cl_2$ (75 mg, 1 mol%) and 2,3-difluorophenyl Bpin (2.88 g, 1.2 equiv., 12.0 mmol) were added and the mixture was stirred at room temperature for 10 minutes. Next, potassium carbonate (5.5 g, 4.0 equiv.) was added and the mixture was stirred and refluxed overnight until TLC analysis indicated the completion of the reaction. The mixture was cooled and poured into a 250 ml separatory funnel and the organic layer was separated. The aqueous layer was extracted with ethyl acetate (60 ml) twice and the combined organic layers were dried with $MgSO_4$. Column chromatography on silica gel (eluted with hexanes) was used to purify the desired product as white crystals after evaporation (1.8 g, 60 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.21 (m, 2H), 6.97 (m, 2H), 6.89 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 164.1 and 161.6 (d, J = 252.6, 2C), 163.9 and 160.9 (d, J = 298.4, 2C), 158.4, 131.1, 122.0, 121.9, 115.8, 113.3, 110.1 (m, 1C), 104.2, 103.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -109.62 (m, 2F), -112.16 (m, 2F). GC/MS: 303.97/305.93 (twin peaks for bromine atom) found 305.07 calc. Melting point: 93-94°C.

2,6,3',5'-Tetrafluorobiphenyl-4-Bpin (**16**)

A mixture of 2,3',5',6-tetrafluoro-4-bromobiphenyl (1.5 g, 5.0 mmol), potassium acetate (2.93 g, 10.0 mmol) in anhydrous DMF (20 ml) was stirred at room temperature under a nitrogen atmosphere for 15 minutes followed by the addition of bis(pinacolato)diboron (1.5 g, 6.0 mmol, 1.2 equiv.) and palladium tetrakis(triphenylphosphine) (56 mg, 0.05 mmol, 1 mol%). The mixture was then heated to 80°C and stirred overnight. TLC analysis indicated the disappearance of the starting material 2,3',5',6-tetrafluoro-4-bromobiphenyl. After cooling to room temperature, the remaining solids were filtered off. The filtrate was condensed by rotary evaporation, redissolved in ethyl acetate (100 ml) then washed with water (3 x 200 ml) and brine (50 ml). The organic layers were dried over magnesium sulfate and condensed to give a light green oil which was purified by column chromatography on silica gel to give a colorless oil after evaporation (1.6 g, 94%). ^{1}H NMR (400 MHz, $CDCl_3$,) δ: 7.07 (dd, ^{1}J = 5.2Hz, ^{2}J = 0.4 Hz, 2H), 6.98 (d, J = 0.4 Hz, 2H), 6.86 (m, ^{1}H). ^{13}C NMR (100 MHz, $CDCl_3$,) δ (ppm): 164.7 and 162.1 (d, J = 263.1, 1C), 163.9 and 161.5 (d, J = 245.4, 2C), 160.8-158.4 (d, J = 239.6, 1C), 131.1, 130.9, 122.8, 122.1, 121.9, 116.1, 115.8, 115.5-115.3 (d, J = 22.4, 1C), 113.5-113.2 (d, J = 33.1, 1C), 110.1, 109.9, 104.4, 103.8, 103.5; ^{19}F NMR (376MHz, $CDCl_3$,) δ (ppm): -109.5 (m, 2F), -112.1 (m, 2F).

3,5,2',6',2",6"-Hexafluoro-[1,1';4',1"]terphenyl (**17**)

In a 100 ml round bottom flask fitted with a magnetic stirbar 2,6-difluoroiodobenzene (2.4 g, 10.0 mmol) was dissolved in a mixture of H_2O (8 ml) and 1,4-dioxane (20 ml) to give a colorless solution. $Pd(dppf)Cl_2$ (75 mg, 1 mol%) and 2,6,3',5'-tetrafluorobiphenyl-4-Bpin (2.88 g, 1.2 equiv., 12.0 mmol) were added to the solution and the mixture was stirred at room temperature for 10 minutes. Next, potassium carbonate (5.5 g, 4.0 equiv.) was added and the mixture was stirred and refluxed for 24 hours until TLC analysis indicated the completion of the reaction. The mixture was cooled and poured into a 250 ml separatory funnel and the organic layer was separated. The aqueous layer was extracted with ethyl acetate (60 ml) twice and the combined organic layers were dried with $MgSO_4$. Column chromatography on silica gel (eluted with hexanes) was used to purify the desired product as white crystals after evaporation (1.4 g, 64 %). Melting point: 216-217°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 7.37 (m, 1H), 7.17 (m, 2H), 7.06 (m, 4H), 6.88 (m, ^{1}H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 164.0-161.6 (d, J = 246.6, 2C), 160.7-158.2 (d, J = 248.4 2C), 130.2, (t, J = 10.4, 2C), 113.7, 112.0, 104.0 (t, J = 25.0, 2C); ^{19}F NMR ($CDCl_3$, 376 MHz) δ (ppm): -109.89 (m, 2F), -114.07 (m, 2F), -114.31 (m, 2F). GC/MS: 338.18 found, 338.25 calc.

3,5,2',6',2",6",2"',6"'-Octafluoro-[1,1';4',1";4",1"']quaterphenyl (**18**)

Route A towards compound **18**

In a 100 ml round bottom flask fitted with a magnetic stirbar 2,3',5',6-tetrafluoro-4'-iodobiphenyl (1.2 g, 3.5 mmol) was dissolved in a mixture of H_2O (4 ml) and 1,4-dioxane (10 ml) to give a colorless solution. $Pd(PPh_3)_4$ (41 mg, 1 mol%) and 2,3',5',6-tetrafluoro biphenyl-4-Bpin (1.6 g, 1.4 equiv., 5.0 mmol) were added to the solution and the mixture was stirred at room temperature for 10 minutes. Next, potassium carbonate (1.92 g, 2.8 equiv.) was added and the mixture was stirred and refluxed for 24 hours until a yellow precipitate was observed in the flask and TLC analysis indicated the disappearance of the starting iodobiphenyl. The mixture was cooled and the precipitate was filtered by gravity and the filtrate poured into a 250 ml separatory funnel and the organic layer was separated. The aqueous layer was extracted with ethyl acetate twice (60 ml) and the combined organic layers were dried with $MgSO_4$. On the other hand, the filtered precipitate was redissolved in toluene and filtered the suspended solid again. The organic layer from extraction was analyzed with TLC again and no major product was found. The toluene solution, however, contained a quite polar molecule on the TLC plate. The toluene was then removed by rotary evaporation to give the product as a light yellow solid (0.4 g, 27%) and melting point is 305.6-306.5°C. ^{1}H NMR (400 MHz, tetrachloroethane-d_2 at 65°C) δ (ppm): 7.45 (m, 1H), 7.32 (m, 4H), 7.16 (m, 4H), 6.98 (t, J = 4.4 Hz, ^{1}H); ^{13}C NMR (100 MHz, tetrachloroethane-d_2 at 65°C) δ (ppm) = 164.1-160.9 (d, J = 311.4, 2C), 163.8-160.7 (d, J = 322.5, 2C), 160.8-158.4 (d, J = 254.0, 4C), 131.4, 130.2, 128.5, 114.2, 113.9, 113.6, 113.3, 112.0, 110.6, 110.3, 110.0, 109.8, 104.0; ^{19}F NMR (376MHz, tetrachloroethane-d_2 at 65°C) δ (ppm): -109.24 (m, 2F), -113.39 (m, 6F); GC/MS: 450.17 found 450.32 calc.

Route B towards compound **18**

4"-Bromo-3,5,2',6',2",6"-hexafluoro-[1,1';4',1"]terphenyl (**19**)

A 200 ml round bottom flask fitted with a magnetic stirbar was charged with 4-bromo-2,6-difluoroiodobenzene (1.6 g, 5.0 mmol) and a mixture of H_2O (12 ml) and 1,4-dioxane (30 ml) to give a colorless solution. Next, $Pd(PPh_3)_4$ (55 mg, 1 mol%) and 2,3',5',6-tetrafluorophenyl-4-Bpin (1.75 g, 1.0 equiv., 5.0 mmol) were added to the solution and the mixture was stirred at room temperature for 10 minutes followed by the addition of potassium carbonate (1.38 g, 2.0 equiv.). This mixture was stirred and refluxed for 24 hours and a white precipitate was formed. TLC analysis indicated the disappearance of 4-bromo-2,6-difluoroiodobenzene and the formation of two new molecules with one in major amount. The mixture was cooled, poured into a 250 ml separatory funnel and extracted with ethyl acetate (60 ml) twice and the combined organic layers were dried with $MgSO_4$. Column chromatography on silica gel eluted with hexanes was used to purify the desired product as a white solid (1.0 g, 48% yield). Melting point: 204.6-205.4°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.29 (m, 2H), 7.15 (m, 4H), 6.93 (s, ^{1}H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 164.2-161.7 (d, J = 247.8, 2C), 161.0-158.4 (d, J = 256.9, 2C), 131.6, 130.4, 122.3, 116.2-115.9 (d, J = 29.5, 1C), 113.9 (m, 1C), 104.2, 103.9 (t, J = 25.1, 1C); ^{19}F NMR (376MHz, $CDCl_3$) δ (ppm): -109.87 (m, 2F), -112.04 (m, 2F), -114.65 (m, 2F); GC/MS: 415.99/417.91 found, 417.14 calc.

Potassium 2,6-difluorophenyltrifluoroborate (**19b**)

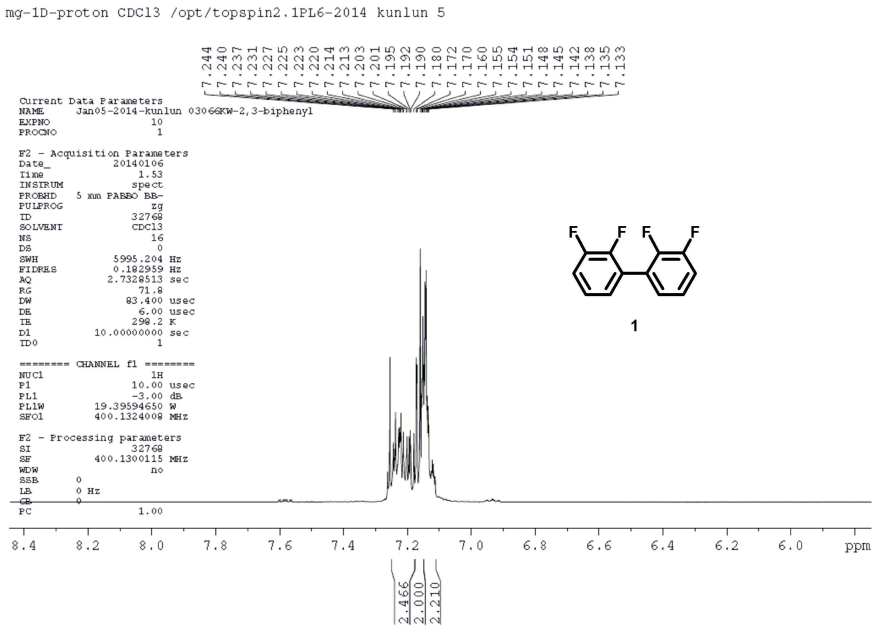
To a stirred suspension of 2,6-difluorophenylboronic acid (2.0 mmol, 315 mg) in methanol (5 ml) was slowly added a solution of KHF_2 (8.0 mmol, 630 mg) in H_2O (5 ml)at room temperature. The resulting mixture was stirred overnight at room temperature and a white precipitate was noticed. The mixture was poured into ice water and the white precipitate was vacuum filtered and washed with H_2O and diethyl ether (each 5 ml x 3). The desired product was obtained quantitatively without further purification. This is a known molecule.[6]

3,5,2',6',2",6",2"',6"'-Octafluoro-[1,1';4',1";4",1"']quaterphenyl (**18**)

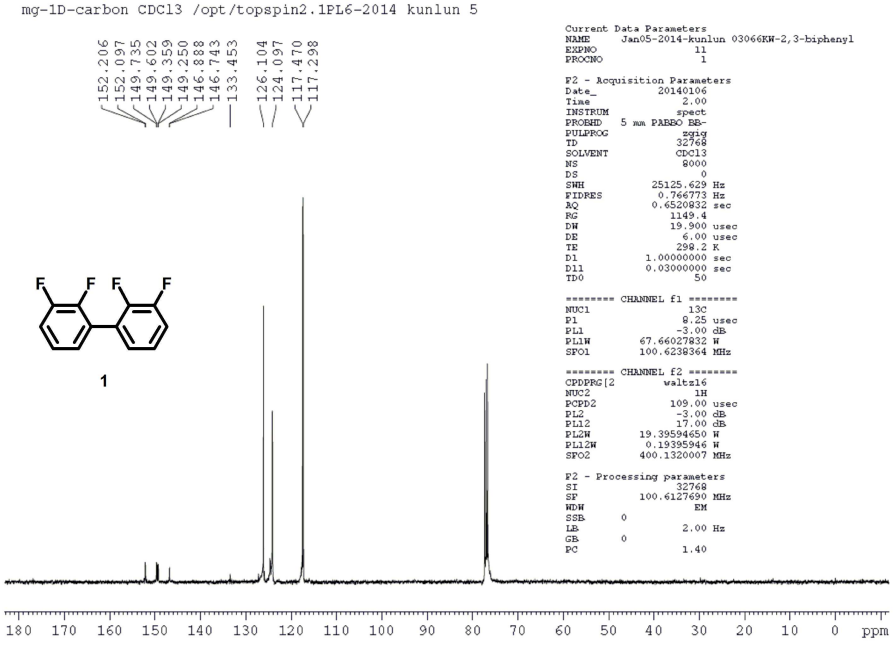
A 200 ml round bottom flask fitted with a magnetic stirbar was charged with 4-bromo-2, 3', 3", 5', 5", 6-hexafluoroterphenyl (417.14 mg, 1.0 mmol) and a mixture of H_2O (6 ml) and 1,4-dioxane (15 ml) to give a colorless solution. Next, $Pd(PPh_3)_4$ (56 mg, 1.0 mol%) and potassium 2,6-difluorophenyl trifluoroborate (330 mg, 1.5 equiv., 1.5 mmol) were added to the solution and the mixture was stirred at room temperature for 10 minutes followed by the addition of potassium carbonate (552 mg, 4.0 equiv.) and this mixture was stirred and refluxed for 48 hours and a white precipitate was formed. TLC analysis indicated the presence of unreacted 4-bromo-2,3',3",5',5",6-hexafluoroterphenyl and the formation of one new substance that was very polar on the bottom and indicated strong fluorescence under UV. After cooling to the room temperature, H_2O (200 ml) was added to the mixture and the resulting grey precipitate was filtered off and washed with H_2O to give a grey crude product. The solids were then boiled with silica gel and K-10 clay in toluene and hot filtered by gravity. The filtrate was then condensed and cooled to crystallize a white solid. This solid was isolated by suction filtration. (192 mg, 43%). Melting point: 305.5-306.5°C. ^{1}H NMR (400 MHz, tetrachloroethane at 65°C) δ (ppm) = 7.45 (m, 1H), 7.32 (m, 4H), 7.16 (m, 4H), 6.98 (t, J = 4.4 Hz, ^{1}H); ^{13}C NMR (100 MHz, tetrachloroethane at 65°C) δ (ppm) = 164.1-160.9 (d, J = 311.4, 2C), 163.8-160.7 (d, J = 322.5, 2C), 160.8-158.4 (d, J = 254.0, 4C), 131.4, 130.2, 128.5, 114.2, 113.9, 113.6, 113.3, 112.0, 110.6, 110.3, 110.0, 109.8, 104.0; ^{19}F NMR (376MHz, tetrachloroethane at 65°C) δ (ppm): -109.24 (d, J = 7.9 Hz, 2F), -113.49 (m, 6F); GC/MS: 450.17 found 450.32 calc.

1.2 ^{1}H and ^{13}C NMR Spectra

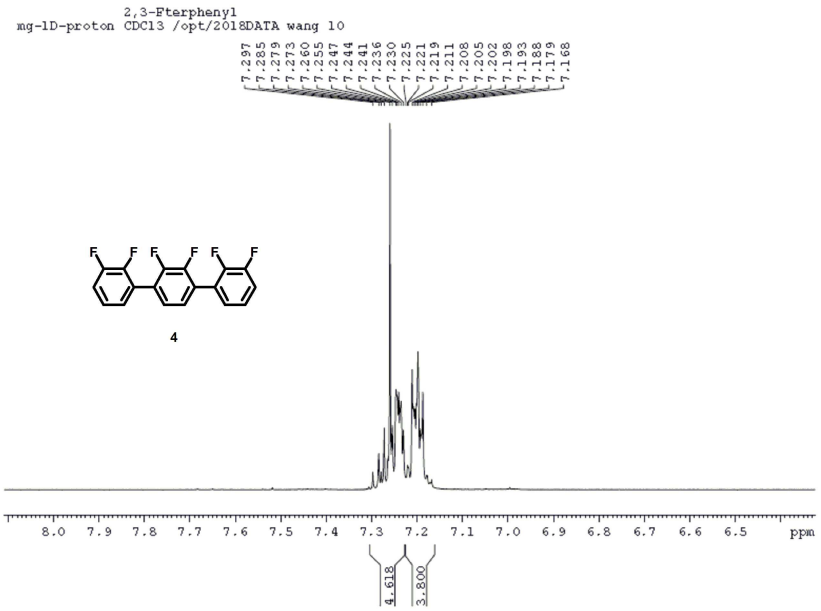
The ^{1}H and ^{13}C NMR spectra of the fluorinated oligomers are provided below.



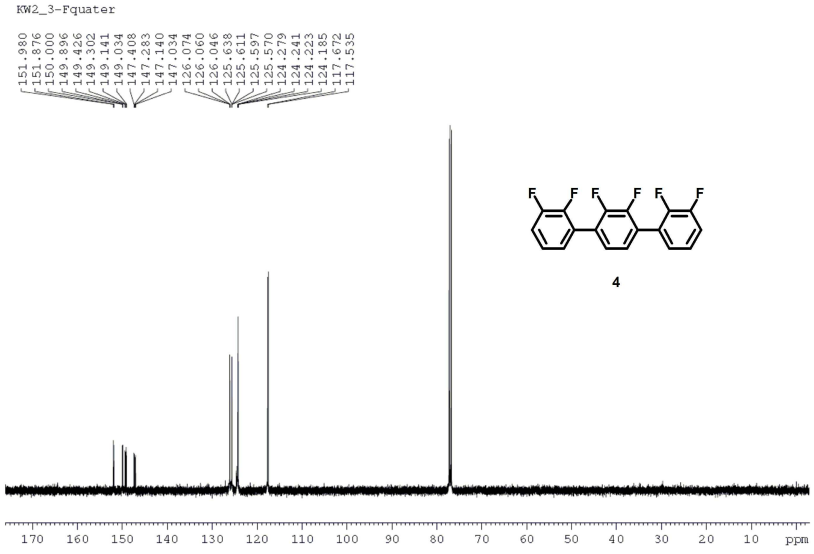
SI Figure 2. ^{1}H NMR spectrum of 2,3-TFBP.



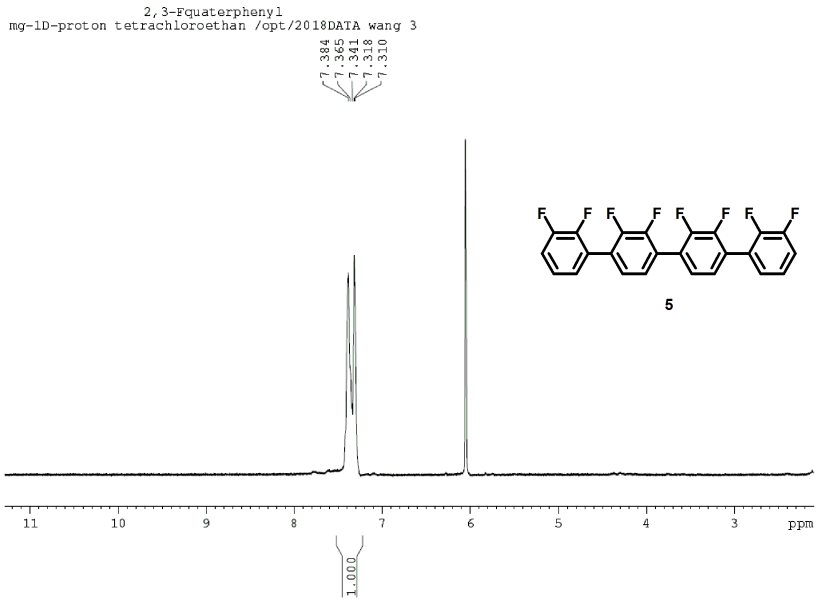
SI Figure 3. ^{13}C NMR spectrum of 2,3-TFBP.



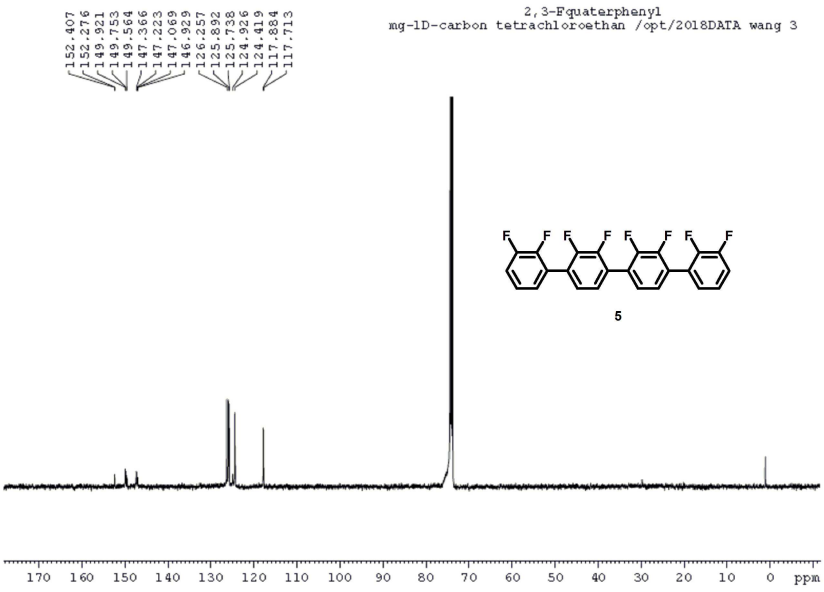
SI Figure 4. ^{1}H NMR spectrum of 2,3-HFTP.



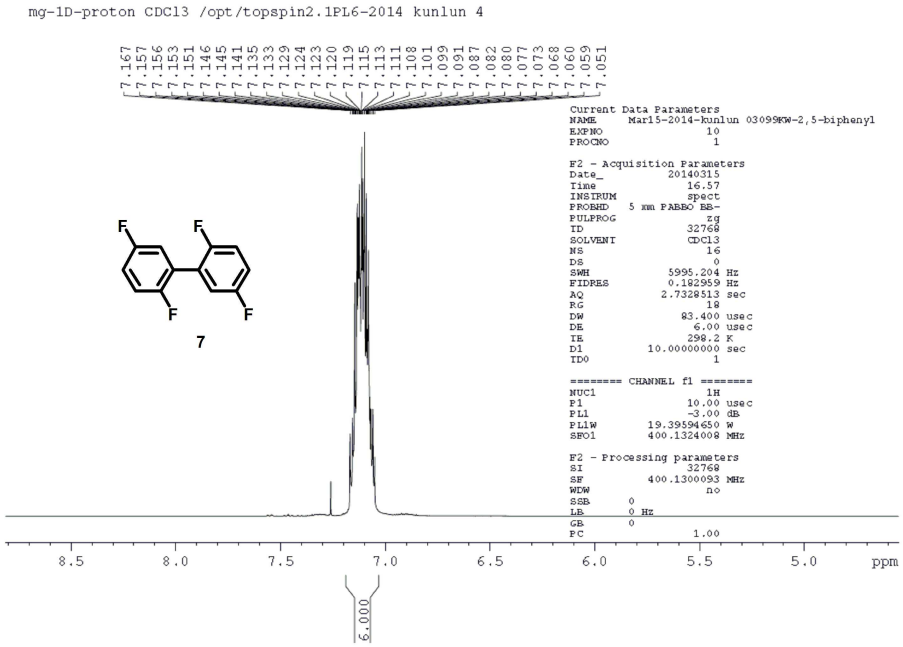
SI Figure 5. ^{13}C NMR spectrum of 2,3-HFTP.



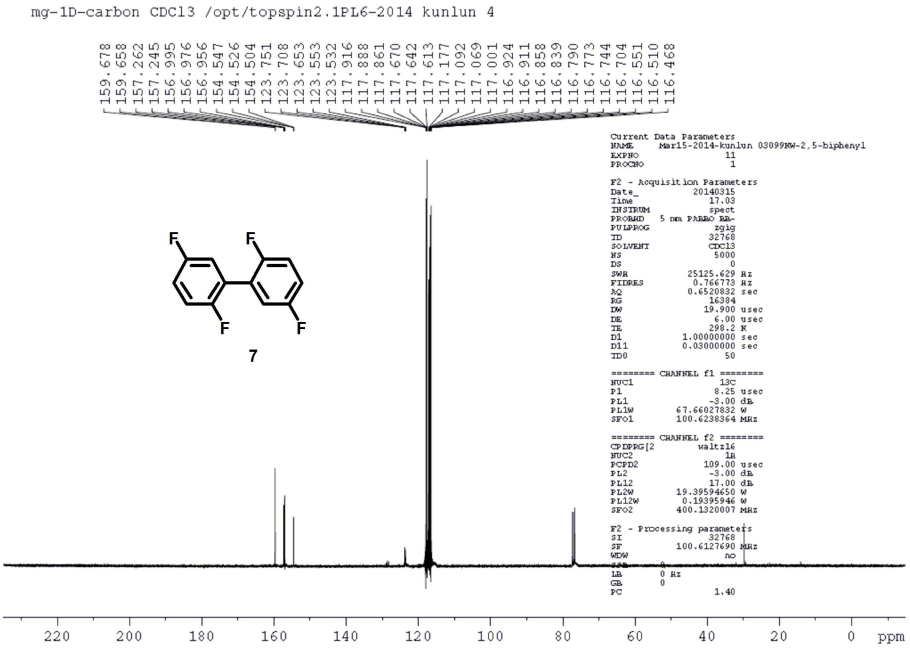
SI Figure 6. ^{1}H NMR spectrum of 2,3-OFQP.



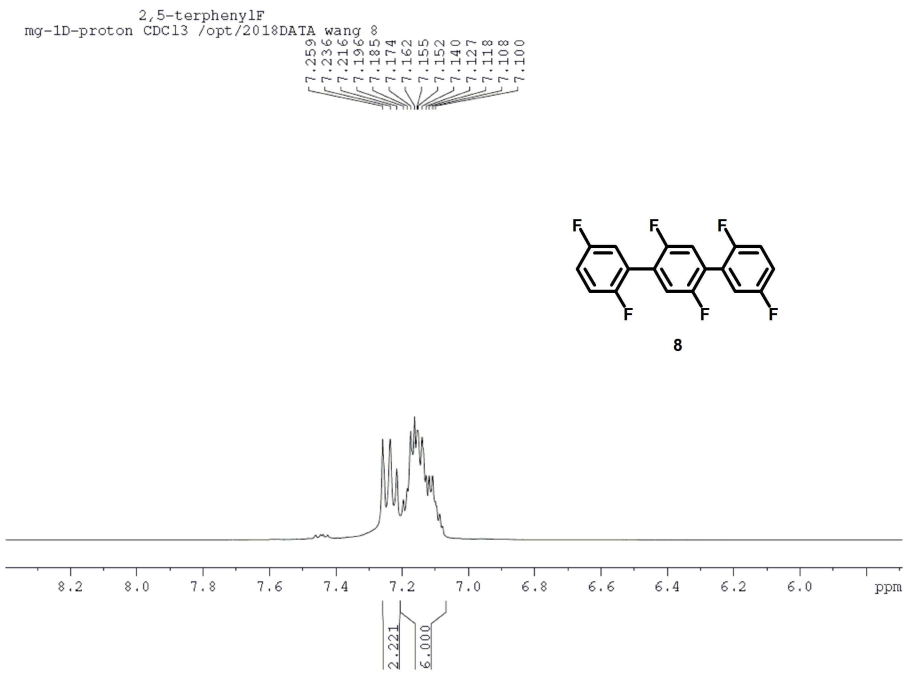
SI Figure 7. ^{13}C NMR spectrum of 2,3-OFQP.



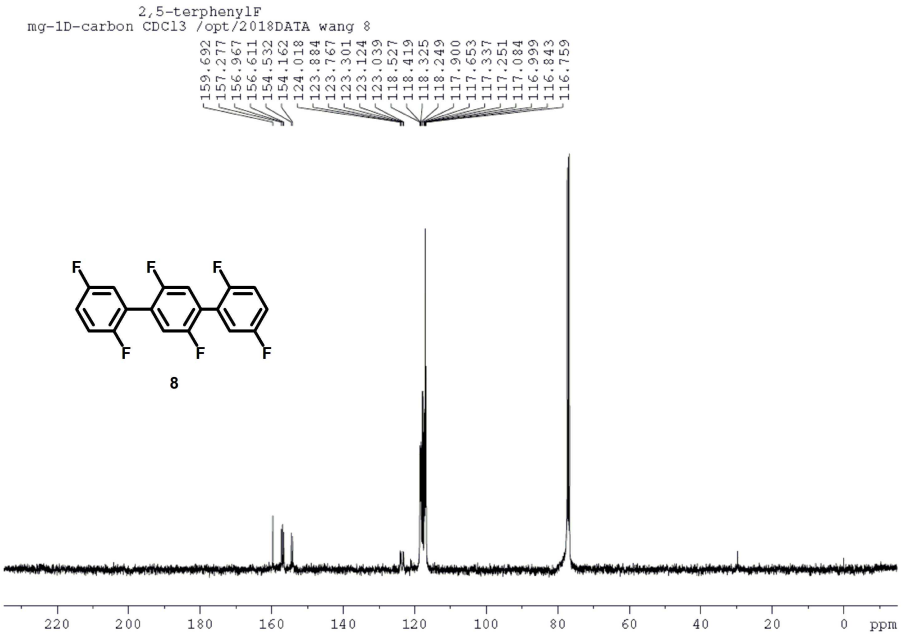
SI Figure 8. ^{1}H NMR spectrum of 2,5-TFBP.



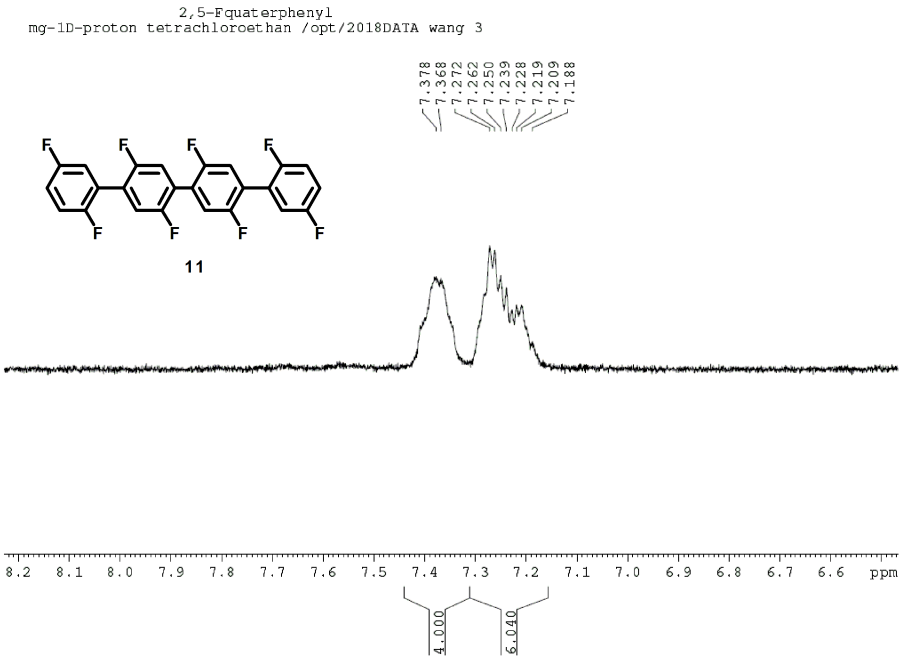
SI Figure 9. ^{13}C NMR spectrum of 2,5-TFBP.



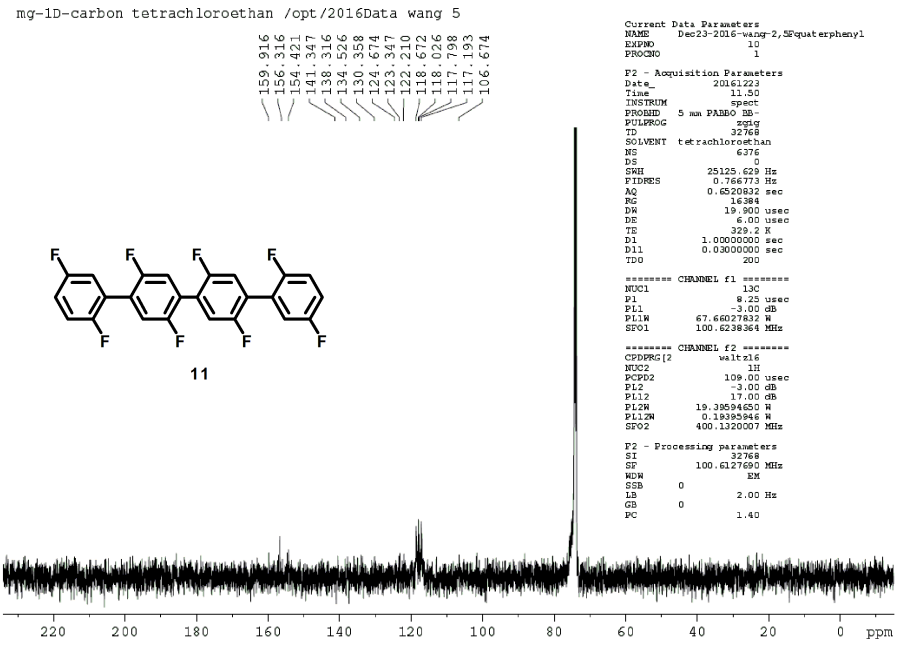
SI Figure 10. ^{1}H NMR spectrum of 2,5-HFTP.



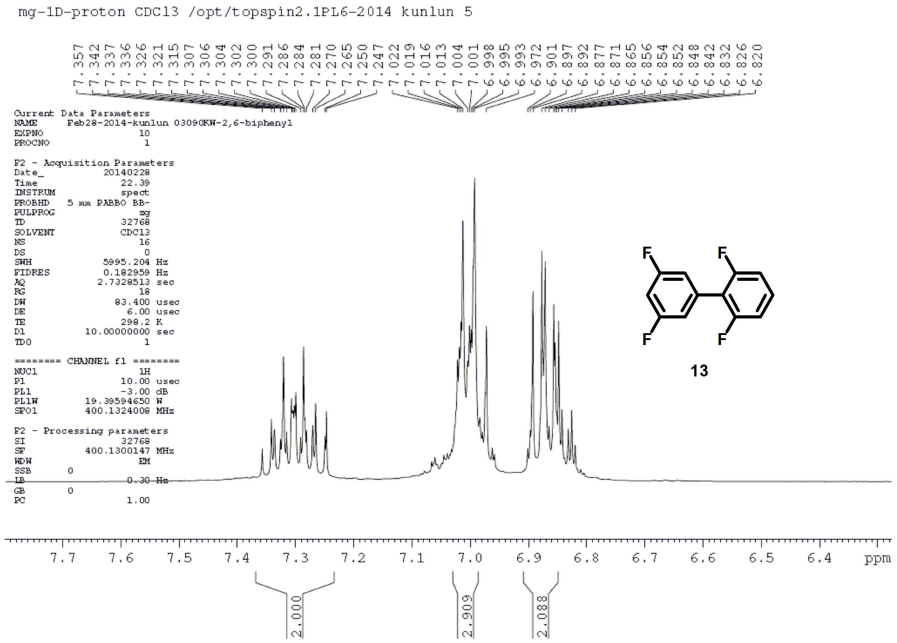
SI Figure 11. ^{13}C NMR spectrum of 2,5-HFTP.



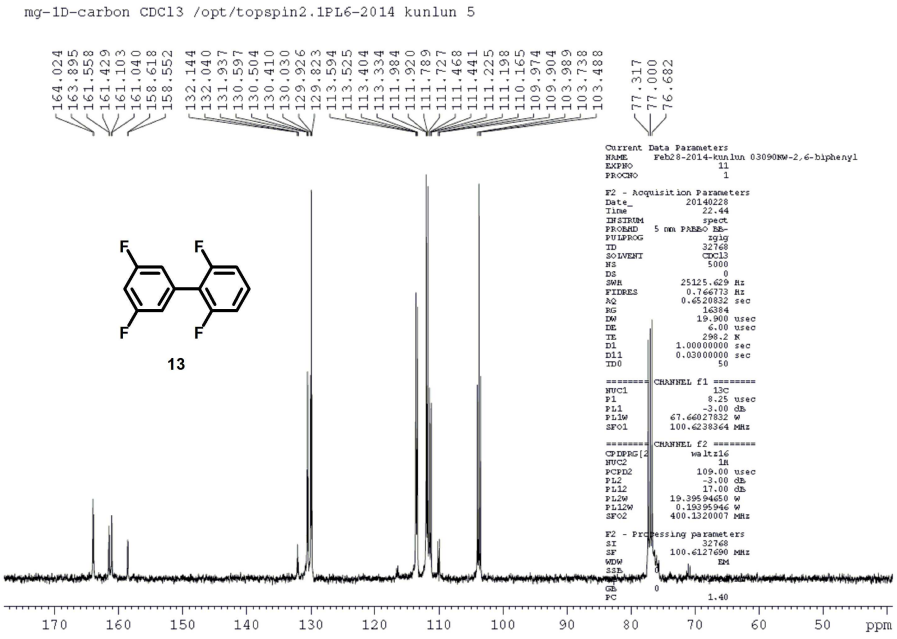
SI Figure 12. ^{1}H NMR spectrum of 2,5-OFQP.



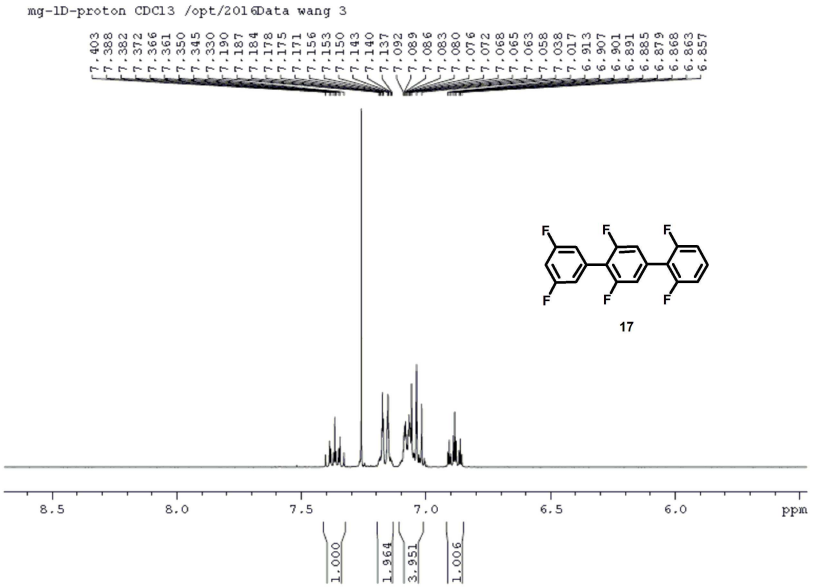
SI Figure 13. ^{13}C NMR spectrum of 2,5-OFQP.



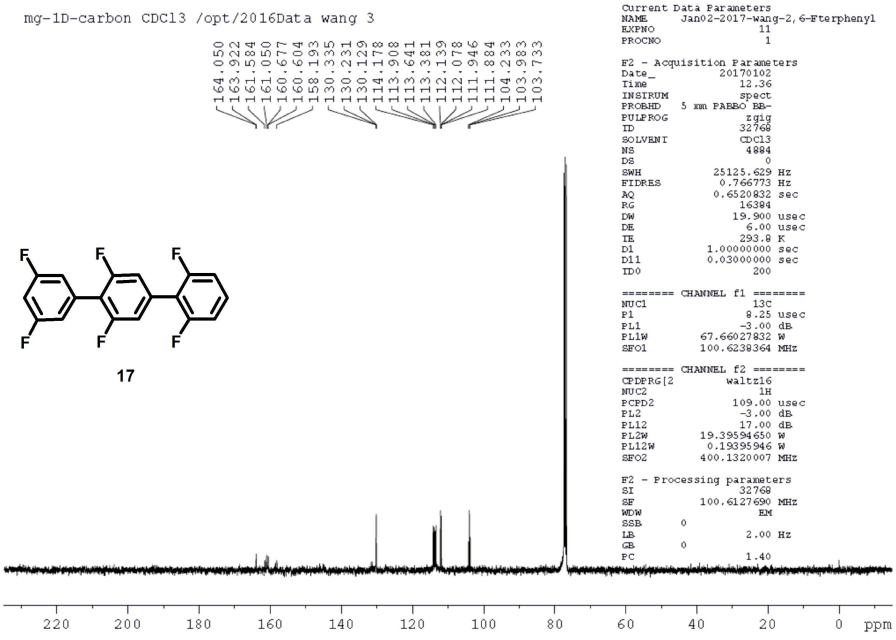
SI Figure 14. ^{1}H NMR spectrum of 2,6-TFBP.



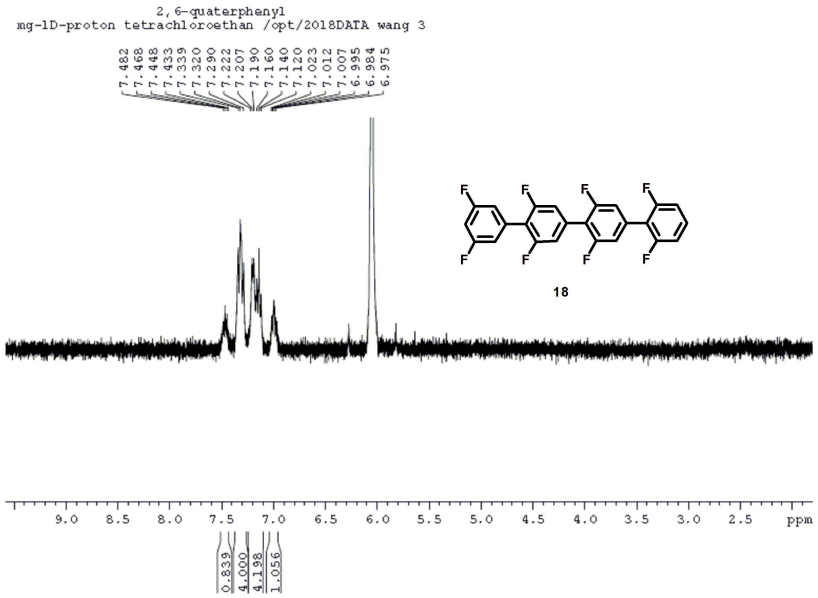
SI Figure 15. ^{13}C NMR spectrum of 2,6-TFBP.



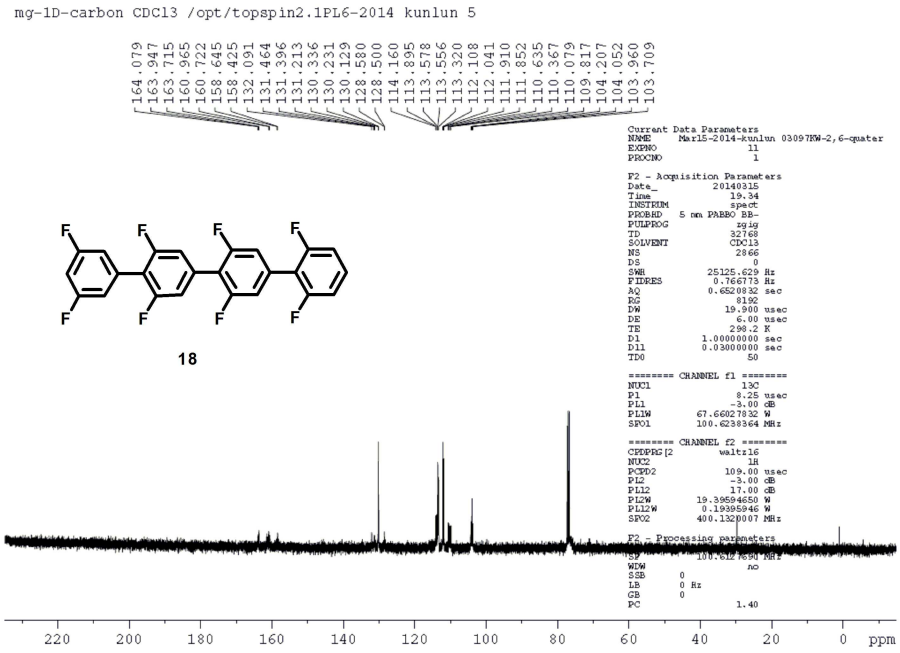
SI Figure 16. ^{1}H NMR spectrum of 2,6-HFTP.



SI Figure 17. ^{13}C NMR spectrum of 2,6-HFTP.



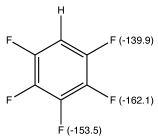
SI Figure 18. ^{1}H NMR spectrum of 2,6-OFQP.



SI Figure 19. ^{13}C NMR spectrum of 2,6-OFQP.

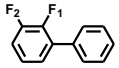
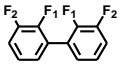
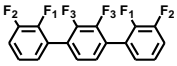
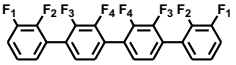
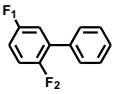
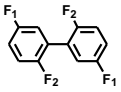
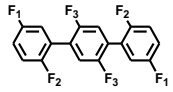
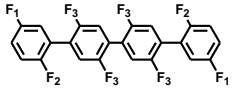
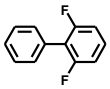
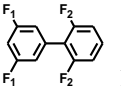
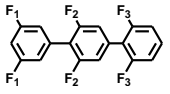
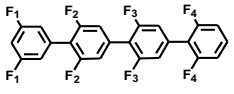
1.3 ^{19}F NMR Spectra

The ^{19}F NMR data for the partially fluorinated oligomers obtained is shown in SI Figure 20. Generally, the ^{19}F NMR chemical shifts for aromatic fluorines range from -100 to -200 ppm.[7] In order to assign all the ^{19}F NMR signals, some partially fluorinated molecules from the literature were selected as references. For instance, the two fluorines on 2,3-difluorobiphenyl appear at -138.0 and -143.8 ppm.[8] In addition, the two fluorines on 2,5-difluorobiphenyl appear at -119.1 and -124.2 ppm.[8] The fluorines in the other isomer, 2,6-difluorobiphenyl, appears at -114.6 ppm.[8] The chemical shifts of the fluorine atoms in the molecules **1**, **4** and **5** (2,3 set) range from 136.7 to 139.4 ppm, which is generally greater than the other two sets of the fluorinated oligophenyls (range from 92.6 to 120.8 ppm). This trend is consistent with the data of the three difluorobiphenyl derivatives mentioned above. Due to the electron withdrawing effect of the adjacent fluorine atom, the fluorine signals of (2,3 set) are deshielded compared to the other two sets. However, it is difficult to assign the signals to each fluorine due to the lack of direct evidence. Although there are hundreds of derivatives with 2,3-difluoro and 2,6-difluoro substitution in literature,[9] there is little fluorine NMR spectral data available for these molecules. We might estimate the chemical shifts by comparison to pentafluorobenzene[9,10] as shown in SI Figure 20. The signal of the para-fluorine actually is located between those of ortho- and meta- fluorines. The data of 2,3,4,5,6-pentafluoro-1,1'-biphenyl is also consistent with this molecule.[11]



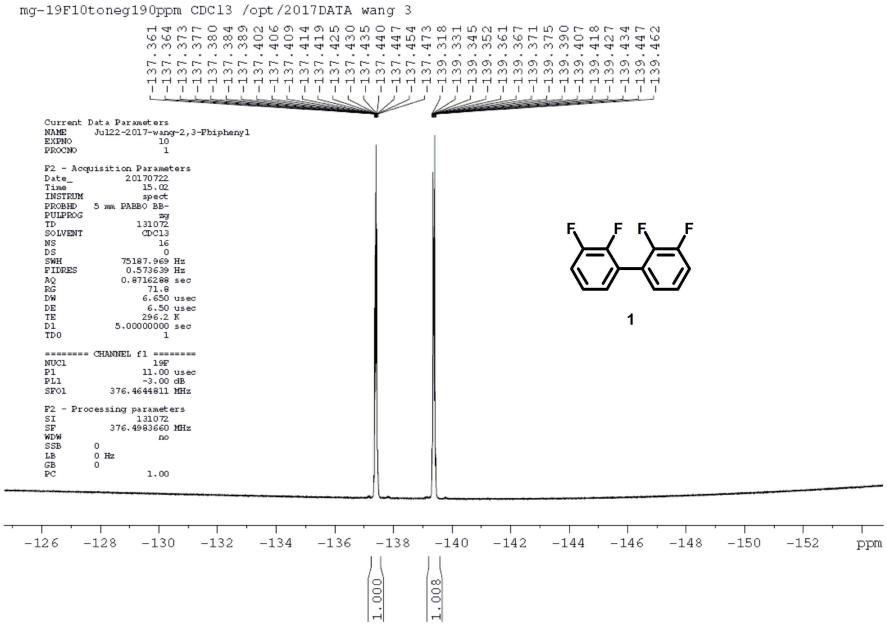
SI Figure 20. The chemical shifts of pentafluorobenzene.

Based on this data and also taking the molecular symmetry into consideration, all the signals are assigned as shown in SI Figure 21. For molecule **1**, the signal at 137.4 ppm should belong to the ortho-fluorines F1 and the signal at 139.4 ppm should belong to the meta-fluorines F_2. For molecule **4**, since the left and ring phenyl rings are located at the para-position, their chemical shift values should be lower than the meta-fluorines. As a result, the signal at 136.7 ppm should belong to the F_3 on the central phenyl ring. For the estimation of the 2,6-difluorophenyl species, we take the electron density of each ring into account. Since this set has a symmetric axis that is parallel to the carbon-carbon δ-bonds, if we look at the molecule structures of molecule **13** in SI Figure 21, the 3',5'-difluoro substitution will have an electro withdrawing effect through the δ-bond, which results in a larger electron density in the 3',5'-difluorophenyl ring (left) than the 2,6-difluorophenyl ring (right). According to the basic knowledge of fluorine NMR, the fluorine of the 3' and 5' position will be shielded compared to the fluorine at 2 and 6 position because it is attached to group that is more electron-rich. As a consequence, we assign the signal of -110.1 ppm, which is upfield, to the fluorines of the 3' and 5' position. Since this electron effect can simply transfer through the δ-bonds, we use the same strategy to assign the signals of molecules **17** and **18**.

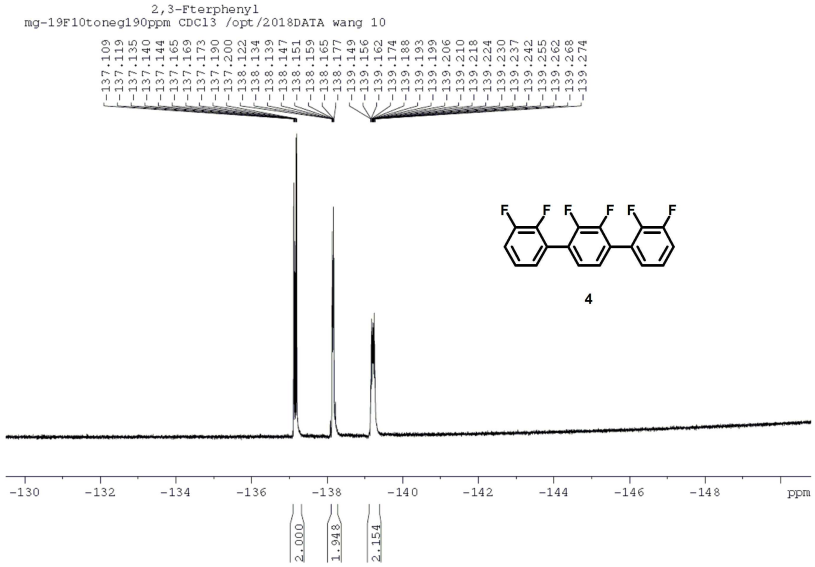
Set	Compound structure/#	^{19}F NMR δ (ppm)
2,3		-138.0 and -143.8 [8]
2,3	 **1**	-137.4 (F_1), -139.4 (F_2).
2,3	 **4**	-137.2 (F_1), -138.1 (F_2), -139.2 (F_3)
2,3	 **5**	-136.7 (F_1), 137.5 (F_3, F_4), 138.7 (F_2)
2,5		-119.1 and -124.2 [8]
2,5	 **7**	-118.9 (F_2), -120.9 (F_1)
2,5	 **8**	-118.6 (F_3), -120.1 (F_2), -120.6 (F_1)
2,5	 **11**	-117.9 (F_3), -119.2 (F_2), -119.8 (F_1)
2,6		-114.6 [8]
2,6	 **13**	-110.1 (F_1), -114.1 (F_2)
2,6	 **17**	-109.9 (F_1), -114.1 (F_2), -114.3 (F_3)
2,6	 **18**	-109.2 (F_1), -113.4 (F_2, F_3, F_4)

SI Figure 21. ^{19}F NMR data of the fluorinated oligomers and some known molecules from the literature.

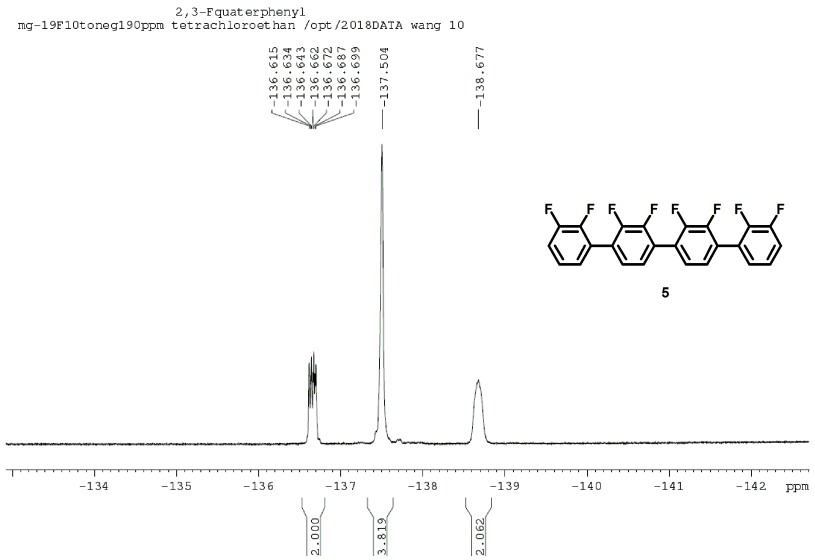
The ^{19}F NMR spectra of the fluorinated oligomers are provided below.



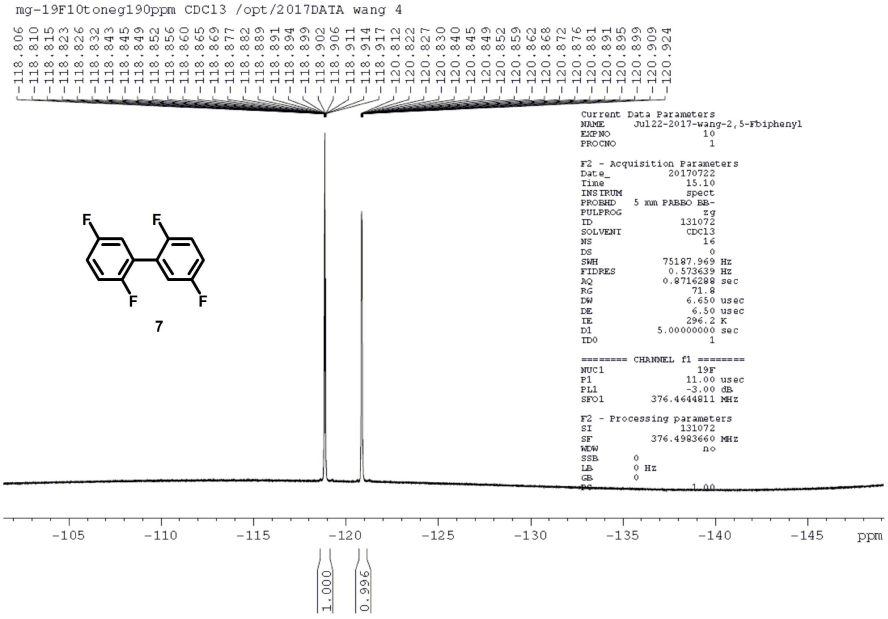
SI Figure 22. ^{19}F NMR spectrum of 2,3-TFBP.



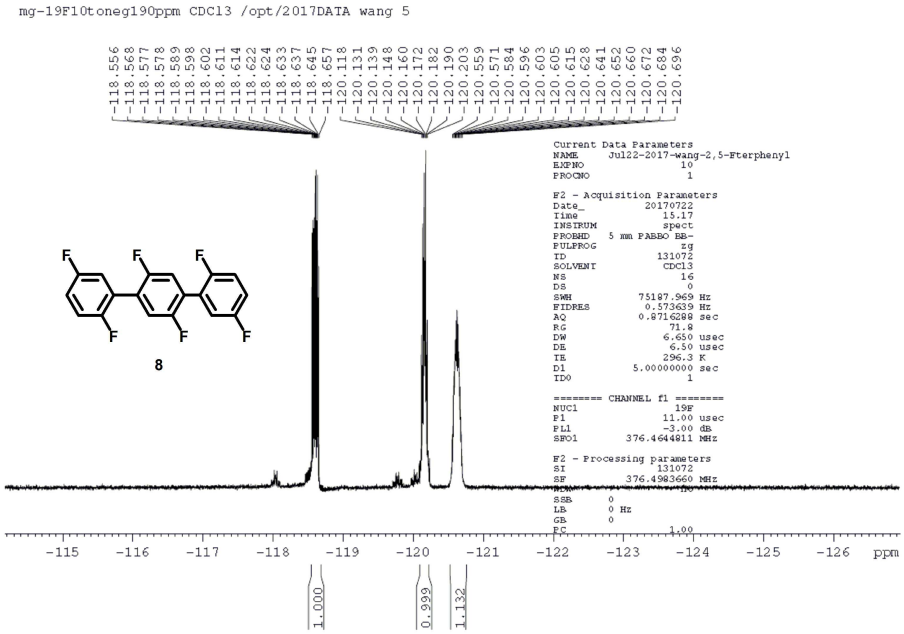
SI Figure 23. ^{19}F NMR spectrum of 2,3-HFTP.



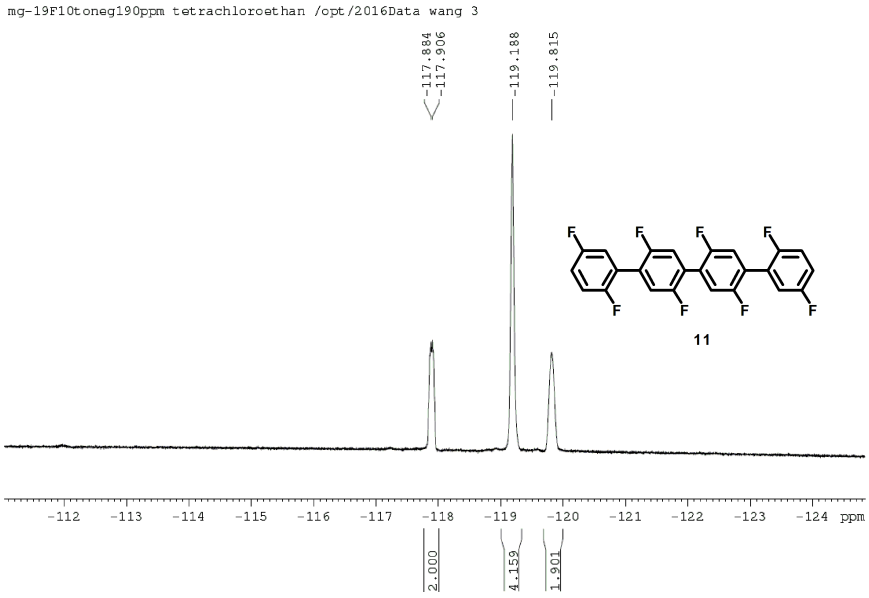
SI Figure 24. ^{19}F NMR spectrum of 2,3-OFQP.



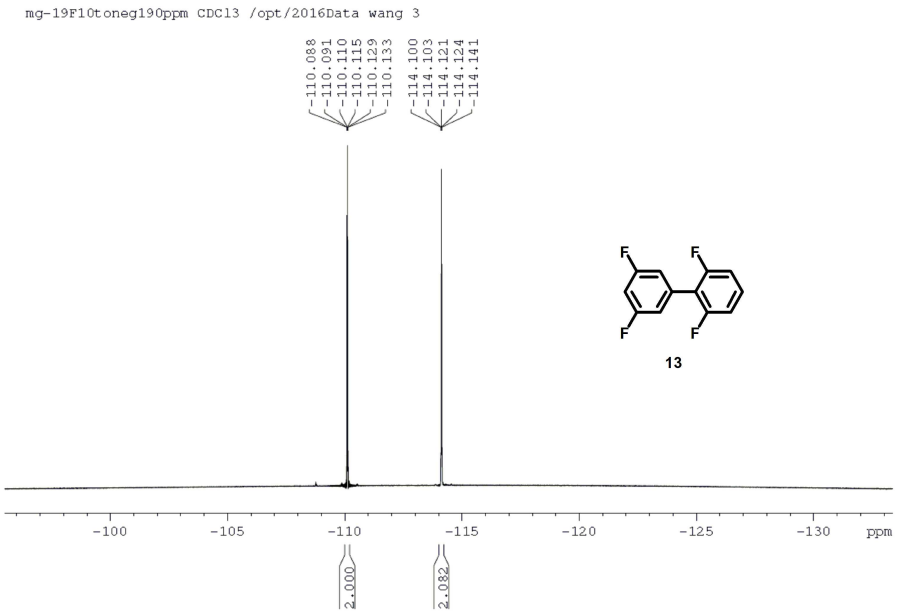
SI Figure 25. ^{19}F NMR spectrum of 2,5-TFBP.



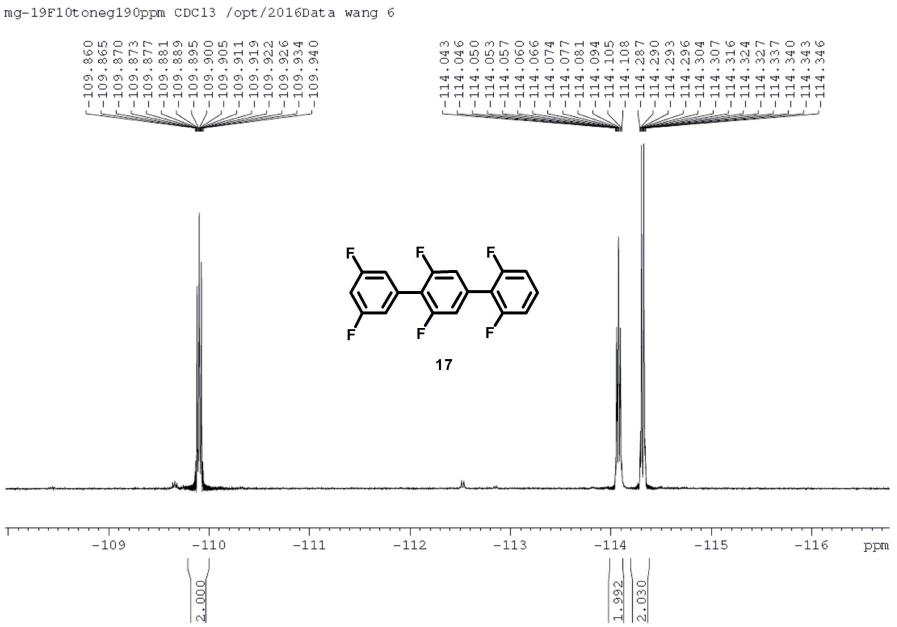
SI Figure 26. ^{19}F NMR spectrum of 2,5-HFTP.



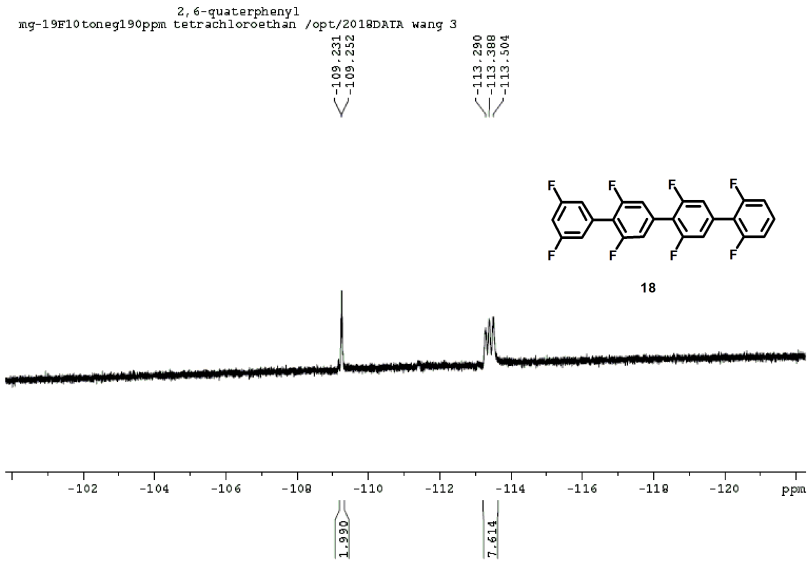
SI Figure 27. ^{19}F NMR spectrum of 2,5-OFQP.



SI Figure 28. ^{19}F NMR spectrum of 2,6-TFBP.



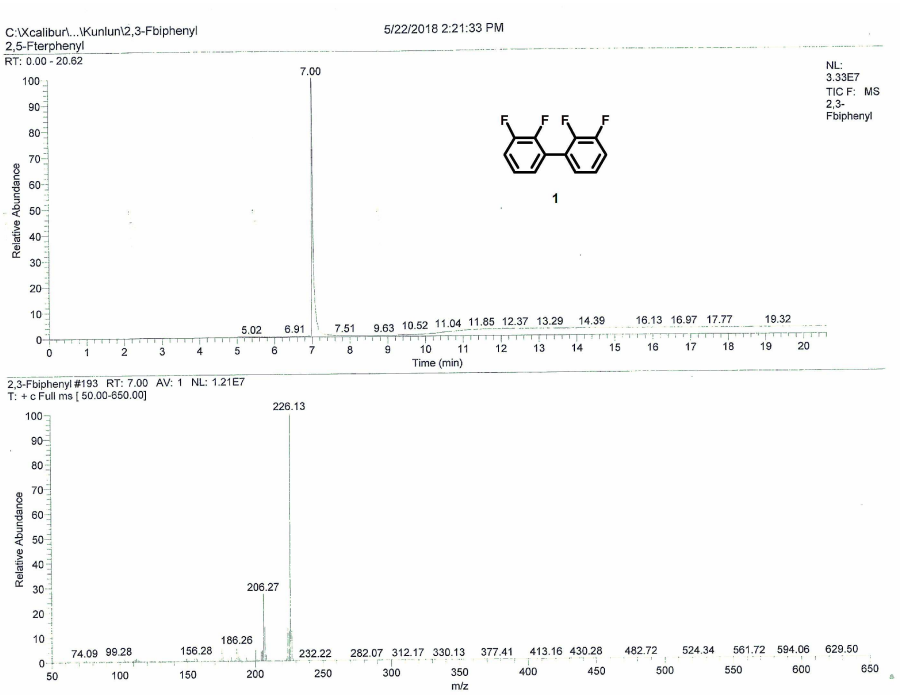
SI Figure 29. ^{19}F NMR spectrum of 2,6-HFTP.



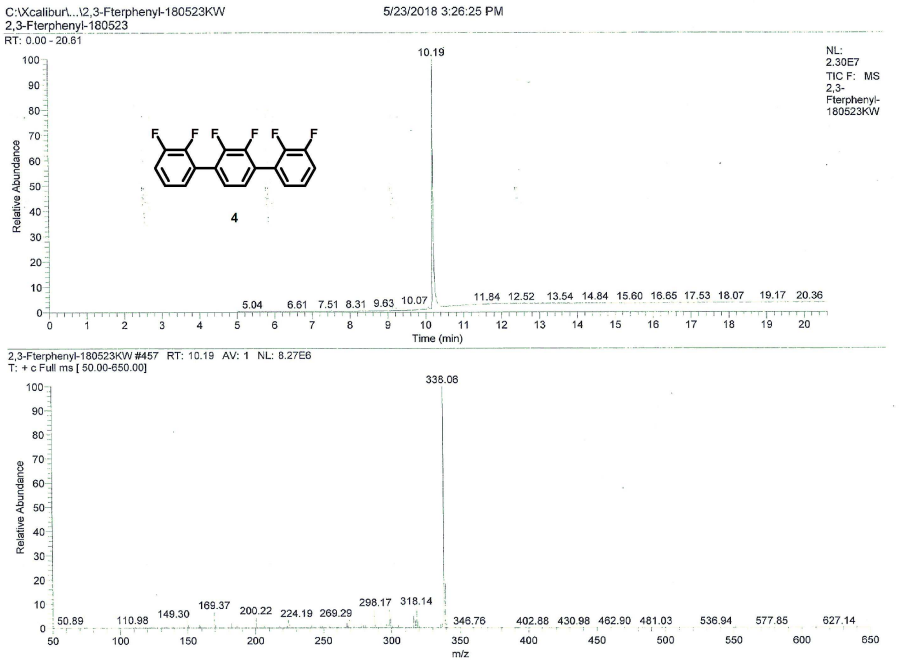
SI Figure 30. ^{19}F NMR spectrum of 2,6-OFQP.

1.4 Mass Spectra

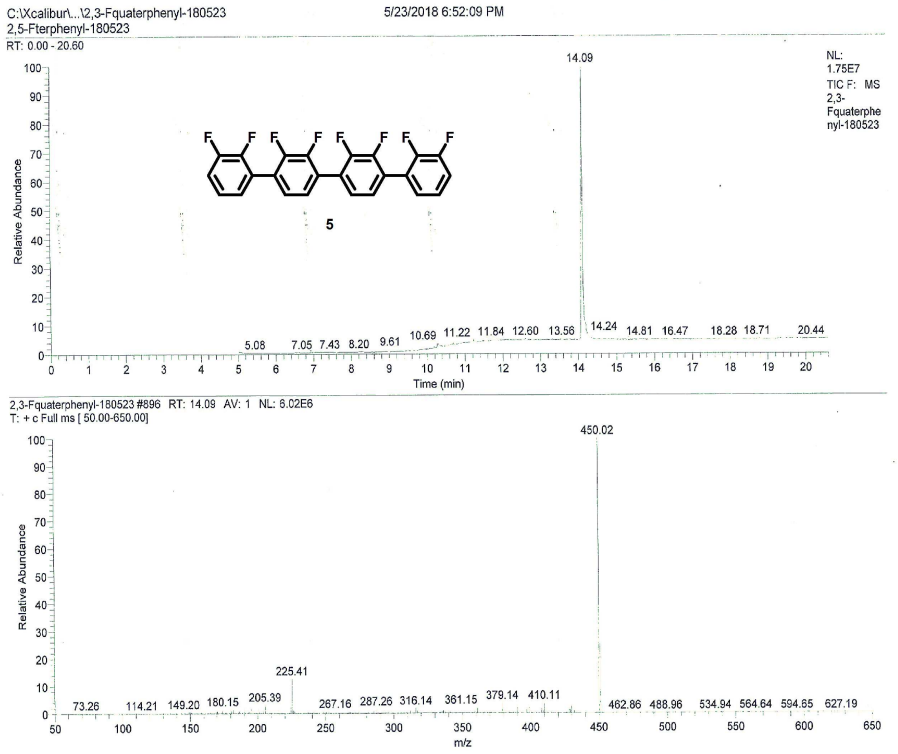
The Mass spectra of the fluorinated oligomers are provided below.



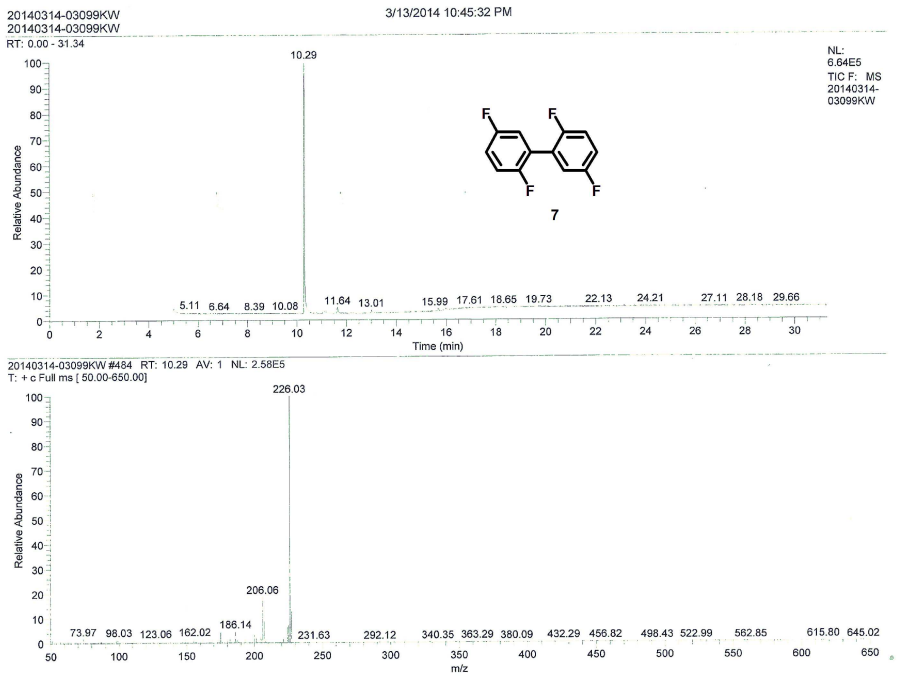
SI Figure 31. Mass spectrum of 2,3-TFBP.



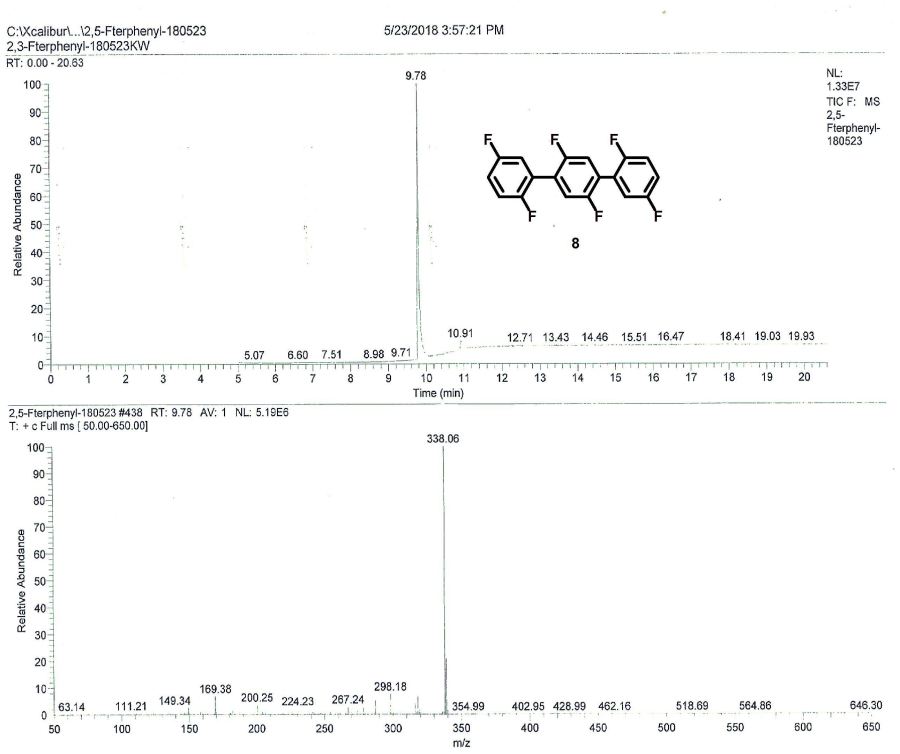
SI Figure 32. Mass spectrum of 2,3-HFTP.



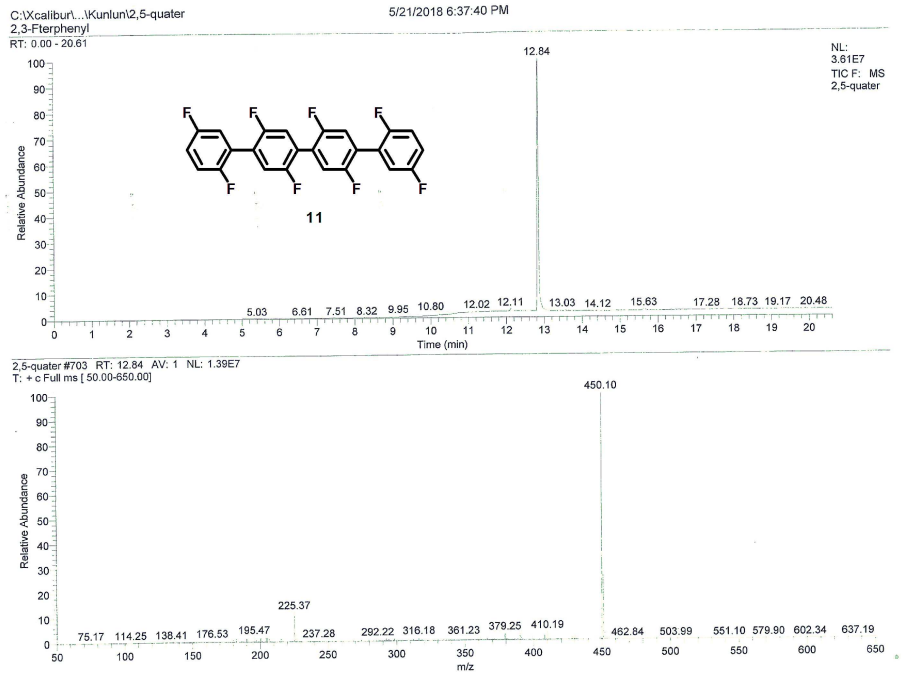
SI Figure 33. Mass spectrum of 2,3-OFQP.



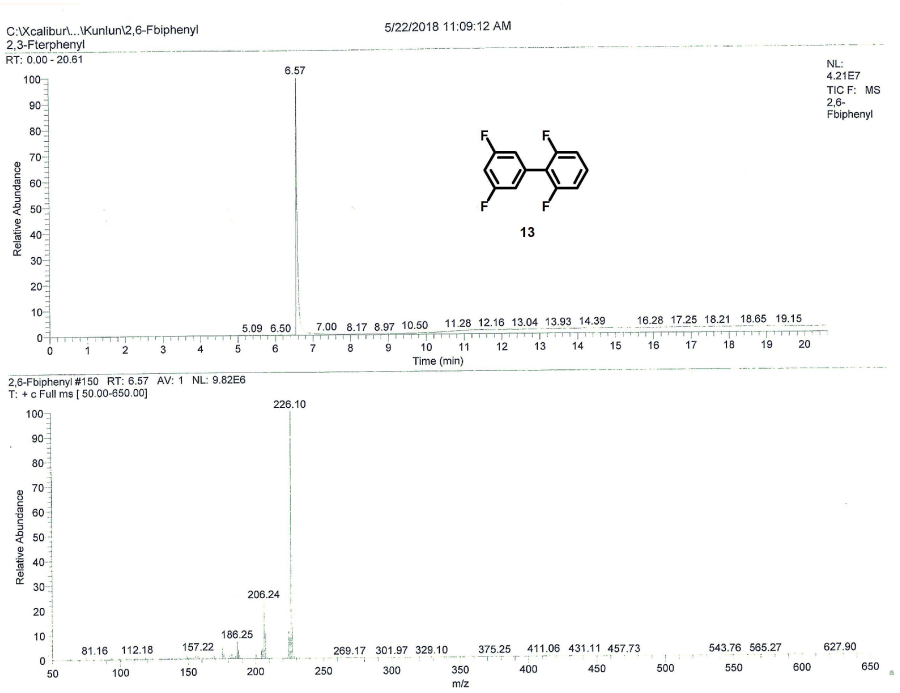
SI Figure 34. Mass spectrum of 2,5-TFBP.



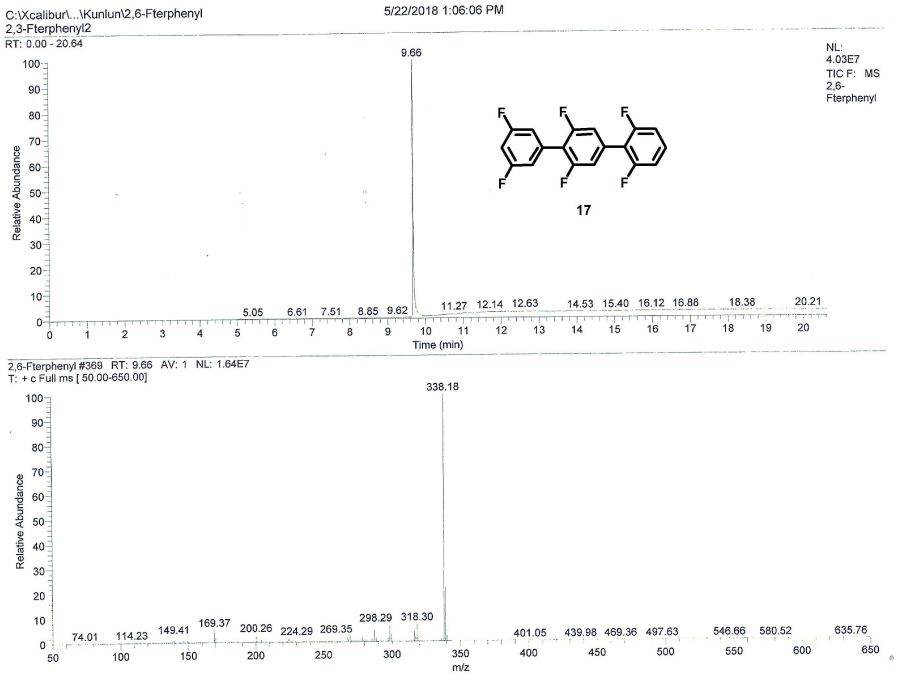
SI Figure 35. Mass spectrum of 2,5-HFTP.



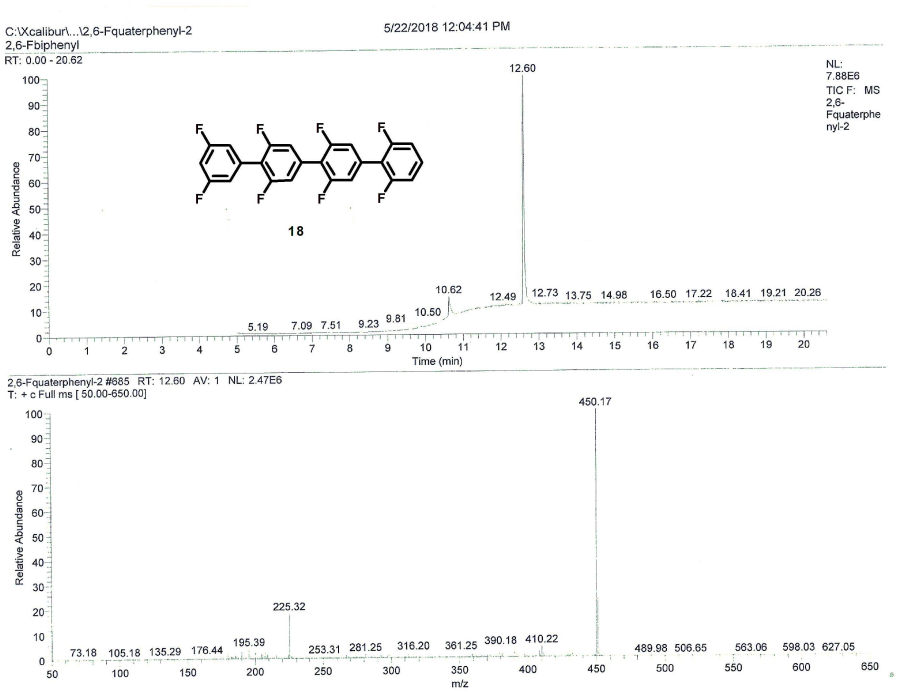
SI Figure 36. Mass spectrum of 2,5-OFQP.



SI Figure 37. Mass spectrum of 2,6-TFBP.



SI Figure 38. Mass spectrum of 2,6-HFTP.



SI Figure 39. Mass spectrum of 2,6-OFQP.

1.5 X-Ray Crystallography

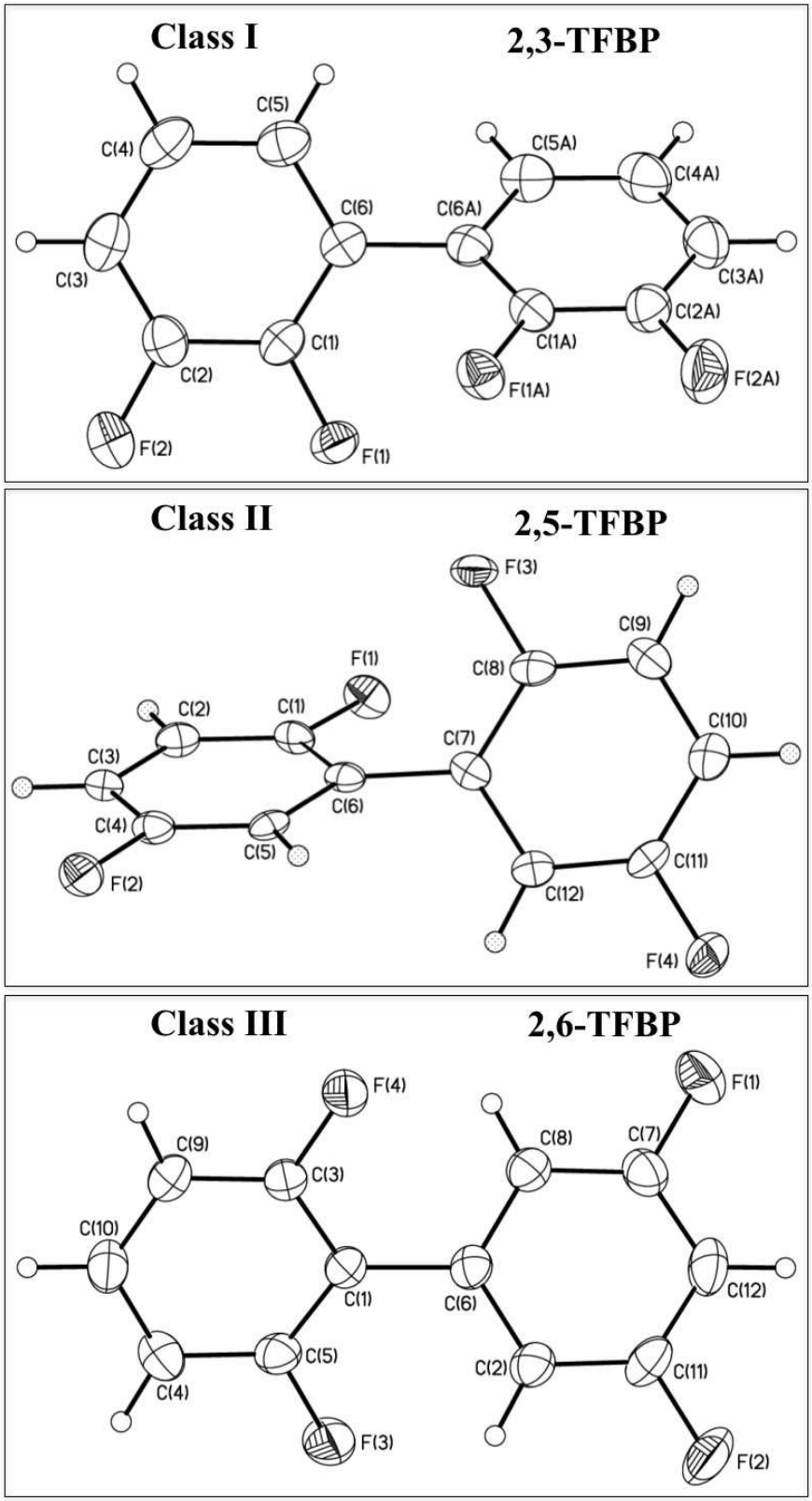
Suitable single crystals for X-ray diffraction studies were obtained for 2,3-TFBP, 2,5-TFBP and 2,6-TFBP. Crystal data for 2,3-TFBP, 2,5-TFBP and 2,6-TFBP were collected by exactly the same method by mounting a crystal onto a thin glass fiber from a pool of Fluorolube^{TM} and immediately placing it under a liquid N_2 cooled stream, on a Bruker AXS diffractometer upgraded with an APEX II CCD detector. The radiation used is graphite monochromatized Mo Kα radiation ($\lambda = 0.7107$ Å). The lattice parameters are optimized from a least-squares calculation on carefully centered reflections. Lattice determination, data collection, structure refinement, scaling, and data reduction were carried out using APEX2 Version 2014.11 software package.[12,13] The data were corrected for absorption using the SCALE program within the APEX2 software package.[12,13] The structure were solved using SHELXT.[14] This procedure yielded a number of the C and F atoms. Subsequent Fourier synthesis yielded the remaining atom positions. The hydrogen atoms are fixed in positions of ideal geometry (riding model) and refined within the XSHELL software package.[15] The final refinement of each molecule included anisotropic thermal parameters on all non-hydrogen atoms was performed using OLEX2-1.2.[16] The crystal data for 2,3-TFBP, 2,5-TFBP and 2,6-TFBP molecule are given in SI Table 1. Crystallographic data for the structures have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication nos: CCDC 1864595-1864597 for 2,3-TFBP, 2,5-TFBP and 2,6-TFBP respectively. Copies of the data can be obtained, free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44-(0)1223-336033 or e-mail: deposit@ccdc.cam.ac.uk).

SI Table 1. Summary of the crystallographic data for 2,3-TFBP, 2,5-TFBP and 2,6-TFBP molecule.

Molecule	2,3-TFBP	2,5-TFBP	2,6-TFBP
Empirical formula	$C_{12}H_6F_4$	$C_{12}H_6F_4$	$C_{12}H_6F_4$
M	226.17	226.17	226.17
Crystal System	Orthorhombic	Orthorhombic	Monoclinic
Space group	Fdd2	Pbca	$P2_1/c$
a/Å	12.1166(19)	7.338(2)	3.7497(6)
b/Å	26.530(4)	12.605(4)	10.4225(17)
c/Å	5.9228(9)	19.886(6)	23.936(4)
α/*	-	-	-
β/*	-	-	90.849(2)
γ/*	-	-	-
V/Å^3	1903.9(5)	1839.4(9)	935.4(3)
ρ_{calcd} (g cm^{-3})	1.578	1.633	1.606
T/K	180(2)	100(2)	180(2)
Z	8	8	4
μ/mm^{-1}	0.146	0.151	0.143
Crystal size (mm)	0.30 x 0.15 x 0.10	0.18 x 0.15 x 0.10	0.20 x 0.15 x 0.05
Reflections collected:			
Total	9190	6878	12487
Unique	834	1618	3259
Final R_1, ωR_2	0.0199, 0.0501	0.0744, 0.1771	0.1982, 0.3739

$$R_1 = \sum \left[|F_0| - |F_c| \right] / \sum |F_0| \, , \omega R_2 = \left[\sum \left[\omega \left(|F_0|^2 - |F_c|^2 \right)^2 \right] / \sum \left[\omega \left(|F_0|^2 \right)^2 \right] \right]^{1/2}$$

$$R = \sum ||F_0| - |F_c|| \, / \sum |F_0| \, , R_\omega = \left[\sum \omega \left(|F_0| - |F_c| \right)^2 \Big/ \sum \omega F_0^2 \right]^{1/2}$$



SI Figure 40. Thermal ellipsoid plots (50% probability) of the 2,3-TFBP, 2.5-TFBP and 2,6-TFBP molecules.

2 Computational Data

2.1 Molecular Orbitals and Electronic Coupling

We explained the electronic coupling coefficients for hole (Γ_h) and electron (Γ_e) transport with the help of simplified molecular orbital pictures. The H / L orbitals are energetically well-separated from H-1 / L+1 orbitals in the case of all *monomer* (see SI Figure 41 – SI Figure 49, left hand side). Therefore, in all cases, the *dimer* orbitals H-1, H, L, and L+1, (SI Figure 41 – SI Figure 49, right hand side) correspond to combinations of the *monomer* orbitals H and L.

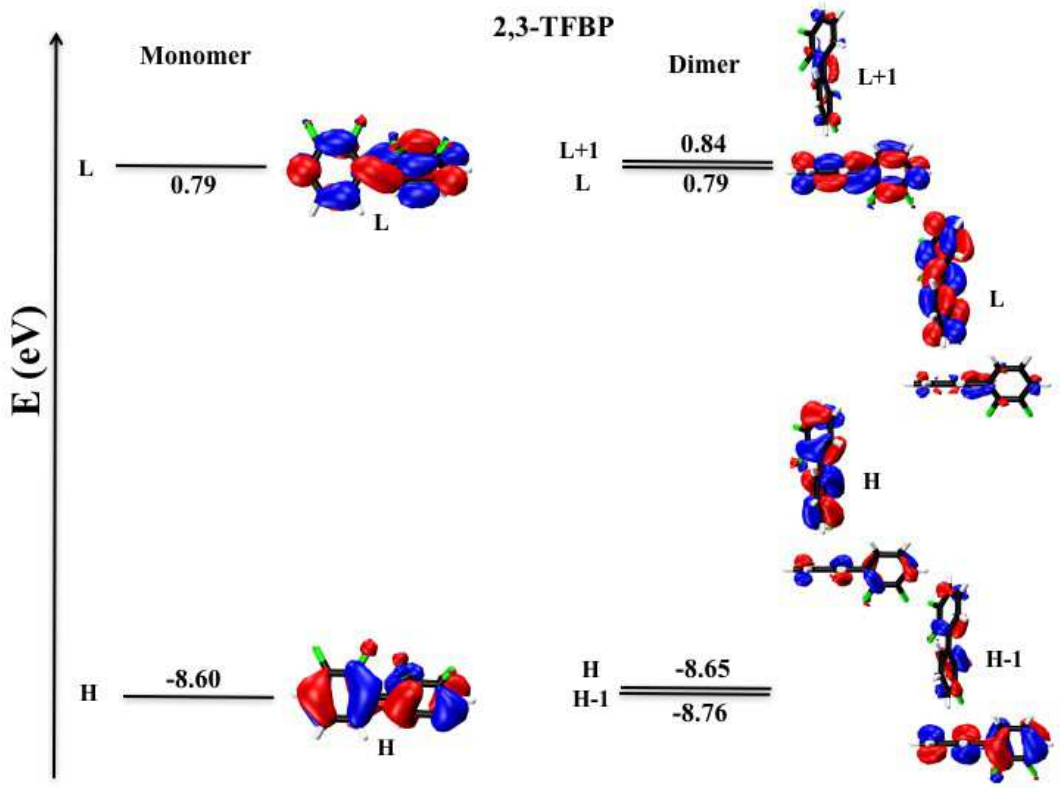
The SI Table 2 indicates that the CDFT-CI method, which gives a good qualitative agreement for symmetrically arranged molecules of Class II and Class III but overestimates for Class I molecules. The crystal structure of Class I molecules is a noncofacial geometry. Therefore each monomer in a dimer experiences a substantially different interactions in Class I molecules. This leads to a symmetry-breaking, lifting the degeneracy between monomer electronic energy levels. The unequal contribution of the two monomer orbitals to the dimer orbitals results in an additional contribution to the energy splitting and eventually increased electronic coupling. The electronic coupling values are omitted in SI Table 2 using orbital energies based method. The Class I symmetry-breaking is well reflected in the dimer MOs, where the H-1, H, L and L+1 are localized on a single monomer (see SI Figure 41 and SI Figure 49), whereas Class II and III molecules typically show fully delocalized dimer orbitals.

Class II systems show smaller electronic coupling for hole transport (Γ_h) and electron transport (Γ_e) whereas Class III systems show significant electronic coupling for hole transport but smaller electronic coupling for electron transport. The dimer model of Class II systems reveals a π stacking arrangement with a lateral shift preferentially along the long molecular axis of the monomers with respect to each other. Since the H-1, H, L and L+1 orbitals are localized in one monomer, this results in a reduced overlap between the lobes of H-1 / H and L / L+1 orbital in the two monomers and makes the smaller electronic coupling of hole and electron transport. The dimer model of Class III systems reveals a π stacking arrangement with delocalized H-1, H, L and L+1 orbitals in monomers. Since the dimer L lobes are oriented along the short molecular axis, this shift results in a reduced overlap of π^* lobes between the two monomers. The situation is slightly different for the lobes of the π bonding H orbitals, which lie along the long molecular axis, thus maintaining a larger overlap for lateral shifts along this axis.

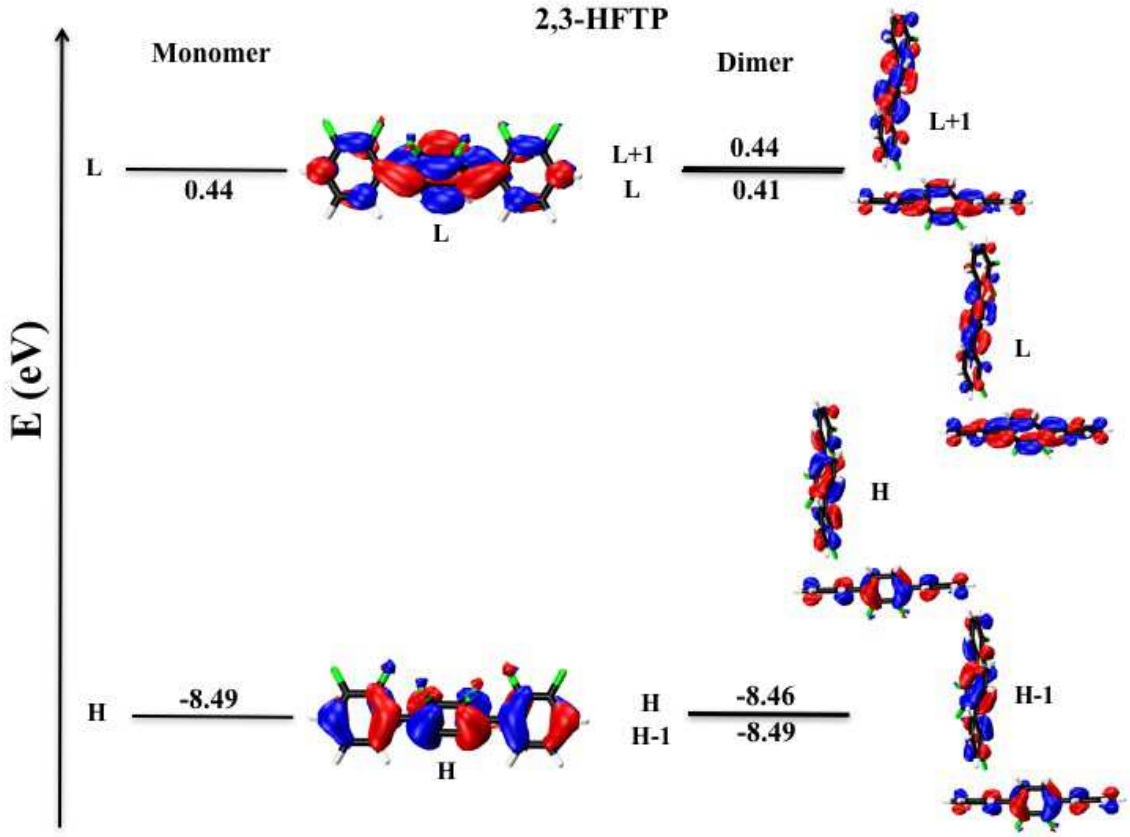
SI Table 2. The electronic coupling coefficients for hole (Γ_h) and electron (Γ_e) transport. CDFT-CI values are compared to orbital energies based values provided in parenthesis.

Molecule	Γ_h [eV]	Γ_e [eV]
	6-31G(d)	
2,3-TFBP	0.013 (—)	0.0045 (—)
2,3-HFTP	0.00098 (—)	0.00041 (—)
2,3-OFQP	0.0022 (—)	0.0012 (—)
2,5-TFBP	0.054 (0.085)	0.040 (0.136)
2,5-HFTP	0.018 (0.054)	0.021 (0.109)
2,5-OFQP	0.0035 (0.027)	0.010 (0.068)
2,6-TFBP	0.216 (0.231)	0.092 (0.122)
2,6-HFTP	0.204 (0.272)	0.083 (0.122)
2,6-OFQP	0.202 (0.272)	0.086 (0.109)
	cc-pVTZ	
2,6-TFBP	0.198 (0.245)	0.097 (0.136)

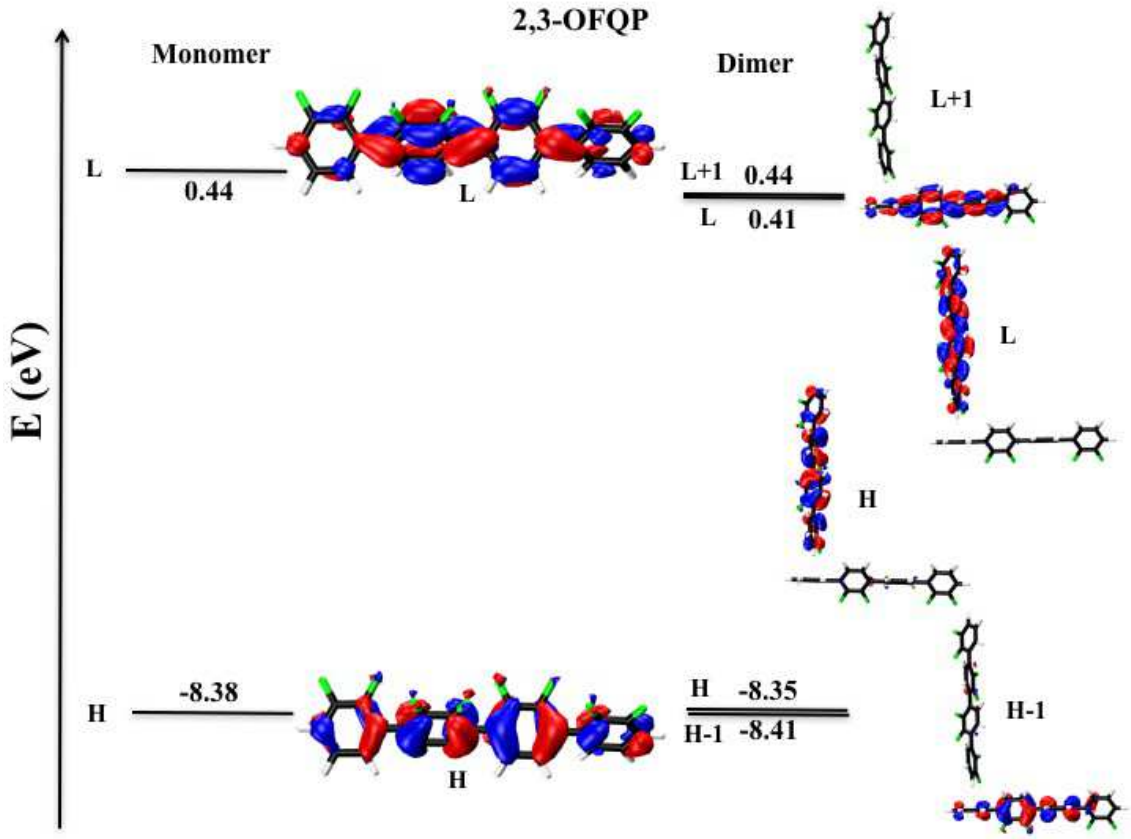
The analysis of molecular orbitals of the fluorinated oligomers are provided below.



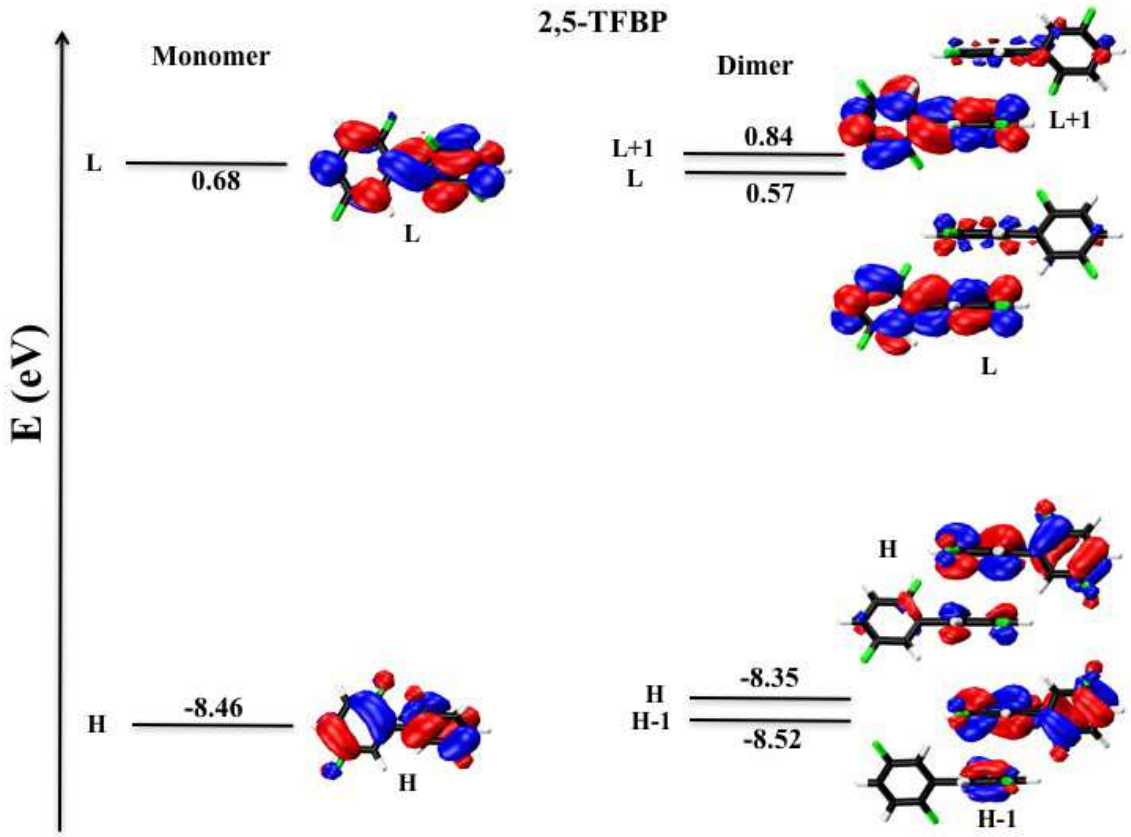
SI Figure 41. The isosurface plots of monomer (left) and dimer (right) molecular orbitals (MOs) for 2,3-TFBP molecule (Class I). The dimer orbitals, H-1, H, L, and L+1, are in all considered cases combinations of the monomer orbitals H and L. Thus, the H-1/H (L/L+1) splitting indicates the hole (electron) transport coupling.



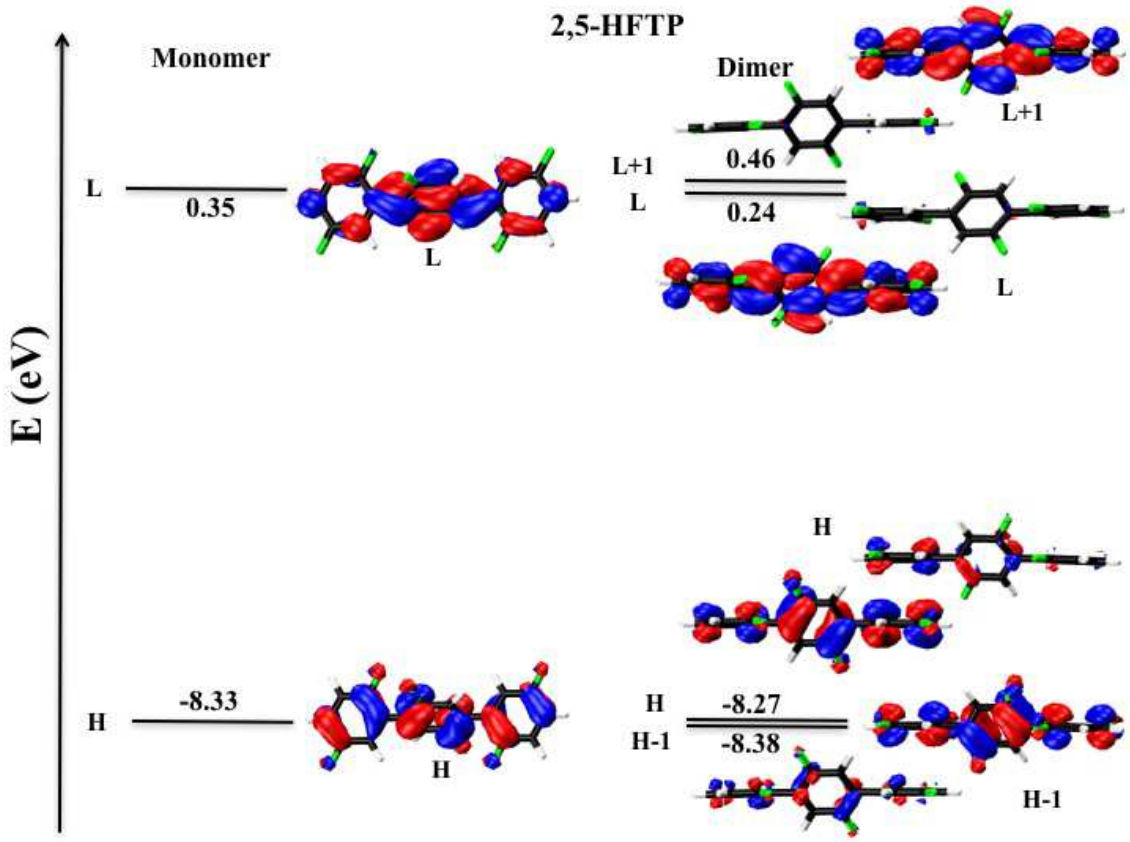
SI Figure 42. The isosurface plots of molecular orbitals (MOs) for 2,3-HFTP molecule (Class I).



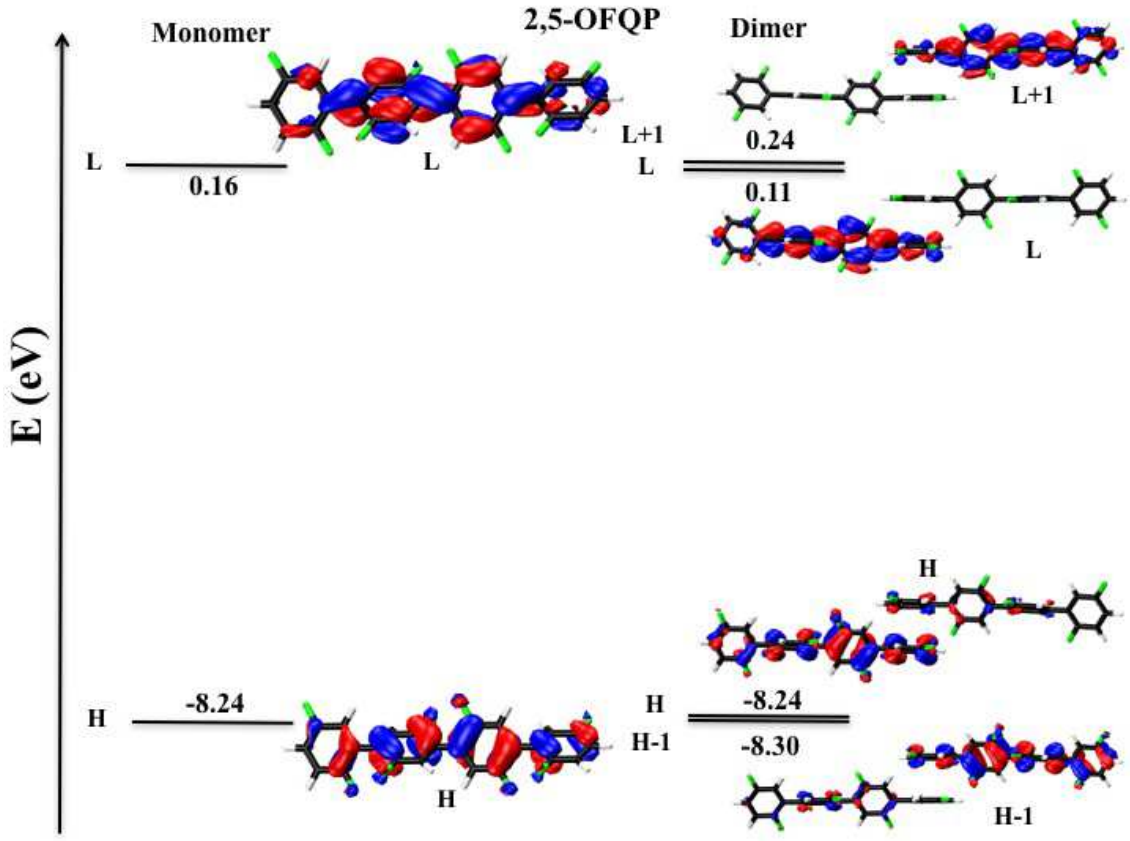
SI Figure 43. The isosurface plots of molecular orbitals (MOs) for 2,3-OFQP molecule (Class I).



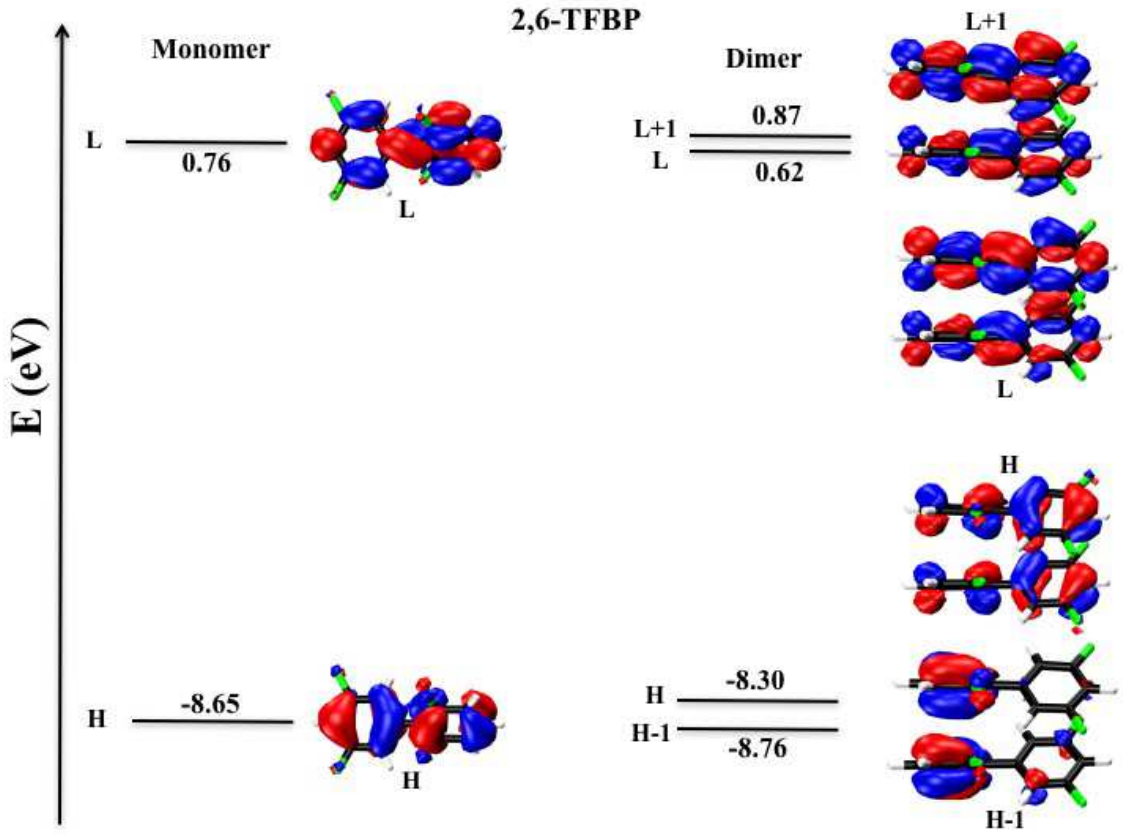
SI Figure 44. The isosurface plots of molecular orbitals (MOs) for 2,5-TFBP molecule (Class II).



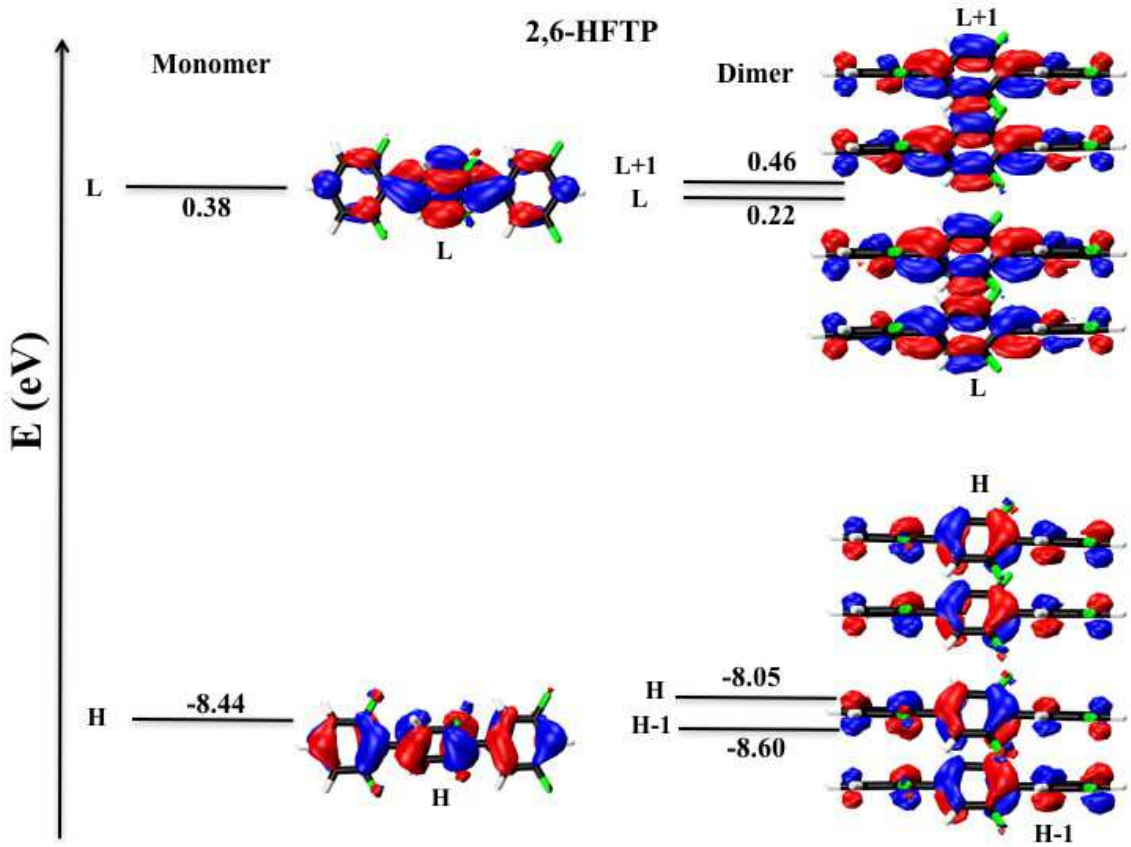
SI Figure 45. The isosurface plots of molecular orbitals (MOs) for 2,5-HFTP molecule (Class II).



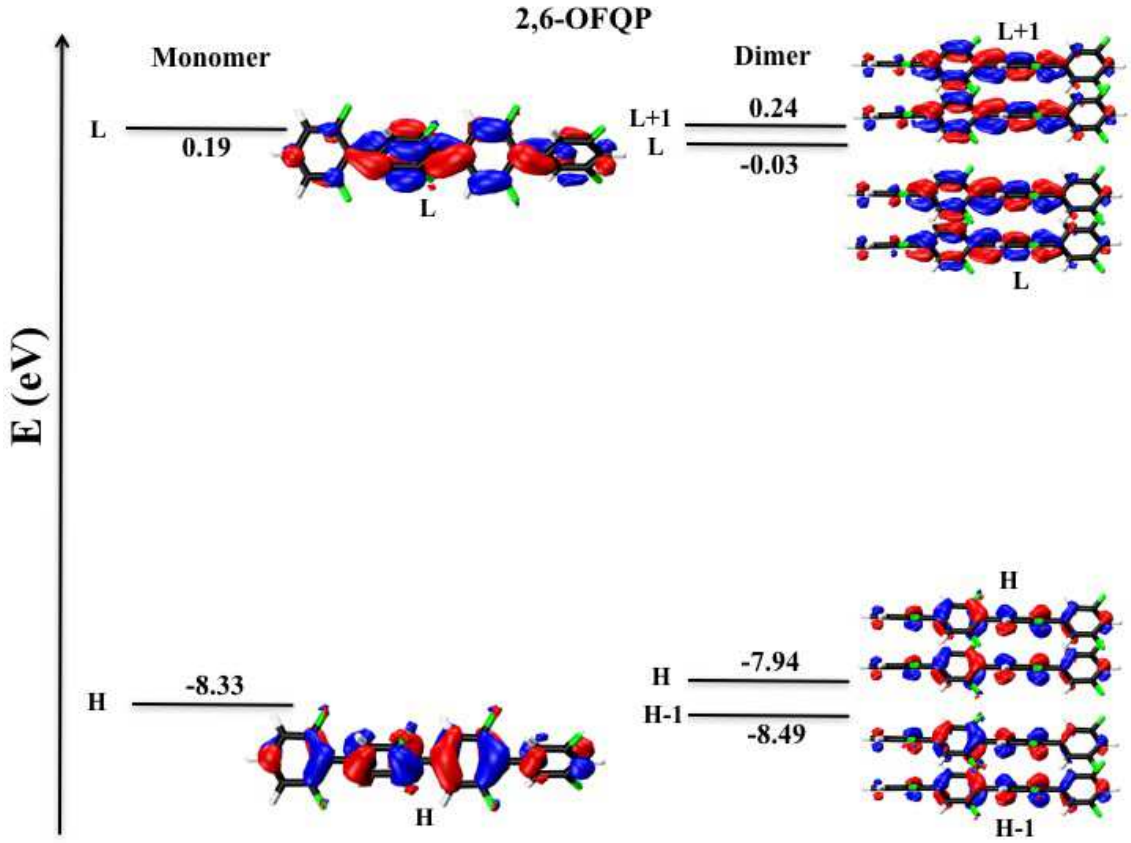
SI Figure 46. The isosurface plots of molecular orbitals (MOs) for 2,5-OFQP molecule (Class II).



SI Figure 47. The isosurface plots of molecular orbitals (MOs) for 2,6-TFBP molecule (Class III).

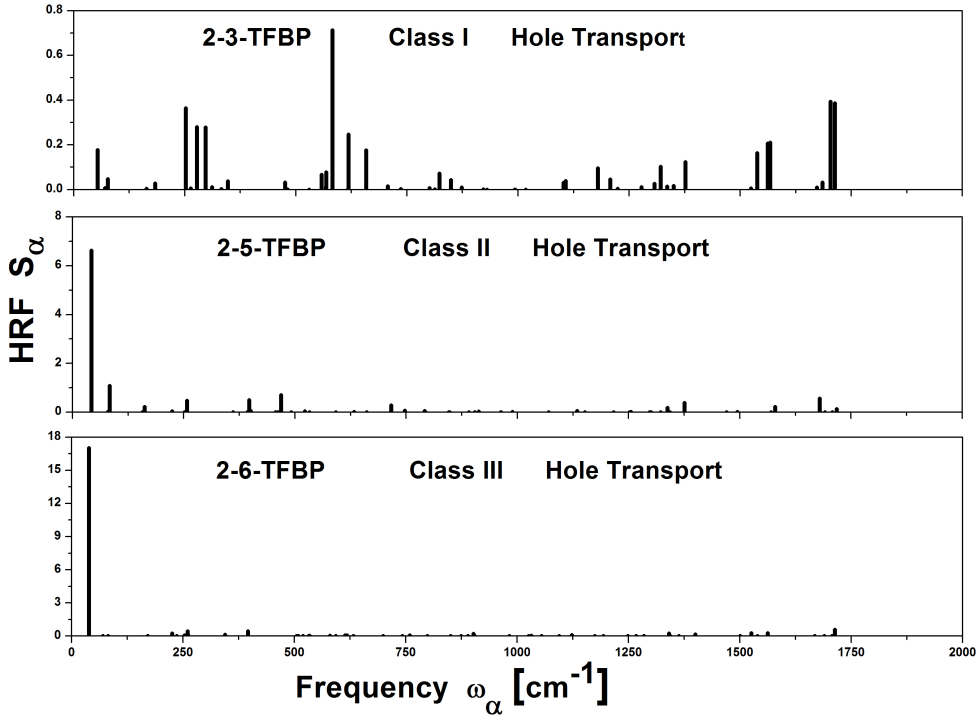


SI Figure 48. The isosurface plots of molecular orbitals (MOs) for 2,6-HFTP molecule (Class III).

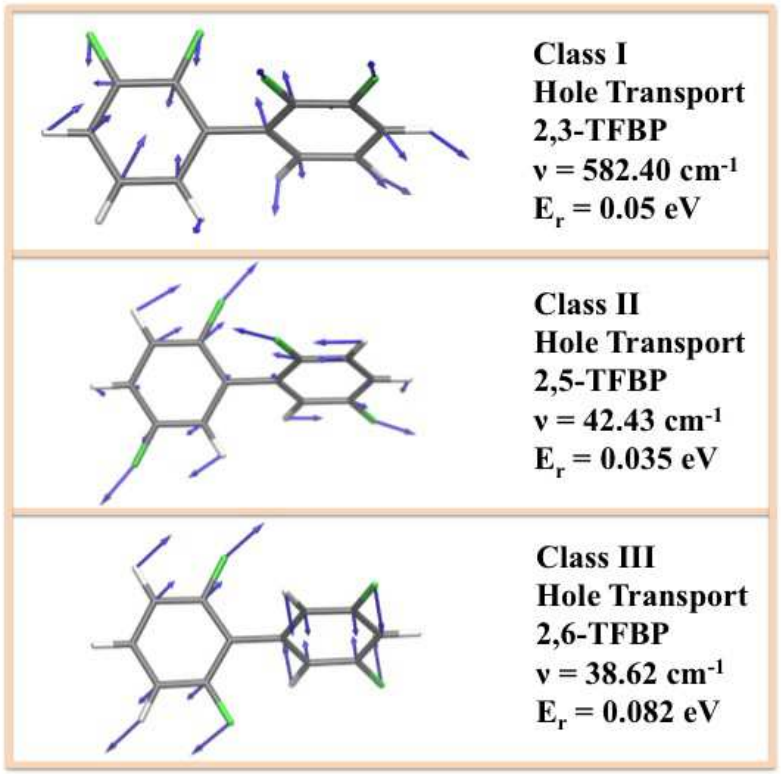


SI Figure 49. The isosurface plots of molecular orbitals (MOs) for 2,6-OFQP molecule (Class III).

2.2 Huang-Rhys Factors, Primary Normal Modes Spectra and Reorganization Energies



SI Figure 50. Huang-Rhys factors S_α (HRFs) for Class I, Class II, and Class III molecules for each normal mode frequency ω_α.



SI Figure 51. The dominant normal modes of hole transport for Class I, Class II, and Class III molecules. The arrows indicate the direction of the normal mode motions. The significant contribution of these modes can be understood within the simplified orbital picture: removing an electron from the dimer HOMO results in a weakening of bonds aligned with the π-lobes causing elongated bond lengths, whereas bonds of low orbital density are strengthened and contract.

SI Table 3. Inner shell reorganization energy (E_r^{in}) calculated with DFT using the ωB97XD functional with a 6-31G(d) and a cc-pVTZ basis set for the monomer model. The reorganization energy is obtained from the direct energy calculation and, in parenthesis, from HRFs calculation as outlined in the manuscript.

Molecule	E_r(h) [eV]	E_r(e) [eV]
6-31G(d)		
2,3-TFBP	0.493 (0.513)	0.738 (0.712)
2,3-HFTP	0.552 (0.496)	0.734 (0.705)
2,3-OFQP	0.541 (0.470)	0.710 (0.637)
2,5-TFBP	0.485 (0.462)	0.724 (0.644)
2,5-HFTP	0.492 (0.457)	0.701 (0.610)
2,5-OFQP	0.500 (0.450)	0.642 (0.592)
2,6-TFBP	0.557 (0.481)	0.782 (0.719)
2,6-HFTP	0.552 (0.454)	0.766 (0.657)
2,6-OFQP	0.566 (0.471)	0.774 (0.670)
cc-pVTZ		
2,6-TFBP	0.641 (0.517)	0.762 (0.720)

2.3 External Reorganization and Solvation Energies

SI Table 4. Comparison of FGR rate constants (Unit: s^{-1}) for hole transport obtained from different Gaussian time windows with time constant $\tau_{sol} = \hbar/\sqrt{k_B T E_r^{ex}}$ (Unit: fs) representing different outer shell solvation energies E_r^{ex} (Unit: meV) in Eq. (1) of the manuscript. A window of 26 fs corresponds to E_r^{ex}=25 meV as used in the manuscript. Windows larger than 80 fs (E_r^{ex}=2.6 meV) would yield erroneous recurrences in the time-dependent integrand of k_{FGR}, see Eq. (1) in the manuscript.

τ_{sol}	80	60	40	26	20	10
E_r^{ex}	2.6	4.6	10.5	25	42	168
Molecule	k_{FGR}	k_{FGR}	k_{FGR}	k_{FGR}	k_{FGR}	k_{FGR}
			6-31G(d)			
2,3-TFBP	4.74×10^{11}	4.46×10^{11}	4.29×10^{11}	4.25×10^{11}	4.30×10^{11}	4.84×10^{11}
2,3-HFTP	1.11×10^{9}	1.12×10^{9}	1.17×10^{9}	1.27×10^{9}	1.39×10^{9}	2.07×10^{9}
2,3-OFQP	7.40×10^{9}	7.50×10^{9}	7.78×10^{9}	8.42×10^{9}	9.13×10^{9}	1.29×10^{10}
2,5-TFBP	6.42×10^{12}	6.48×10^{12}	6.67×10^{12}	7.07×10^{12}	7.48×10^{12}	9.43×10^{12}
2,5-HFTP	6.84×10^{11}	6.91×10^{11}	7.13×10^{11}	7.60×10^{11}	8.09×10^{11}	1.05×10^{12}
2,5-OFQP	2.55×10^{10}	2.58×10^{10}	2.67×10^{10}	2.86×10^{10}	3.06×10^{10}	4.02×10^{10}
2,6-TFBP	8.59×10^{13}	8.69×10^{13}	8.97×10^{13}	9.59×10^{13}	1.02×10^{14}	1.34×10^{14}
2,6-HFTP	9.62×10^{13}	9.73×10^{13}	1.00×10^{14}	1.07×10^{14}	1.13×10^{14}	1.44×10^{14}
2,6-OFQP	6.89×10^{13}	6.98×10^{13}	7.23×10^{13}	7.81×10^{13}	8.43×10^{13}	1.16×10^{14}
			cc-pVTZ			
2,6-TFBP	4.93×10^{13}	4.99×10^{13}	5.17×10^{13}	5.59×10^{13}	6.05×10^{13}	8.50×10^{13}

SI Table 5. Comparison of FGR rate constants (Unit: s^{-1}) for electron transport obtained from different Gaussian time windows with time constant $\tau_{sol} = \hbar/\sqrt{k_B T E_r^{ex}}$ (Unit: fs) representing different outer shell solvation energies E_r^{ex} (Unit; meV) in Eq. (1) of the manuscript. A window of 26 fs corresponds to $E_r^{\rm ex}$=25 meV as used in the manuscript. Windows larger than 80 fs ($E_r^{\rm ex}$=2.6 meV) would yield erroneous recurrences in the time-dependent integrand of $k_{\rm FGR}$, see Eq. (1) in the manuscript.

τ_{sol}	80	60	40	26	20	10
E_r^{ex}	2.6	4.6	10.5	25	42	168
Molecule	$k_{\rm FGR}$	$k_{\rm FGR}$	$k_{\rm FGR}$	$k_{\rm FGR}$	$k_{\rm FGR}$	$k_{\rm FGR}$
			6-31G(d)			
2,3-TFBP	4.40×10^{9}	4.47×10^{9}	4.68×10^{9}	5.18×10^{9}	5.78×10^{9}	1.02×10^{10}
2,3-HFTP	3.10×10^{7}	3.15×10^{7}	3.30×10^{7}	3.67×10^{7}	4.12×10^{7}	7.58×10^{7}
2,3-OFQP	5.30×10^{8}	5.39×10^{8}	5.63×10^{8}	6.21×10^{8}	6.91×10^{8}	1.18×10^{9}
2,5-TFBP	7.06×10^{11}	7.17×10^{11}	7.47×10^{11}	8.20×10^{11}	9.05×10^{11}	1.46×10^{12}
2,5-HFTP	2.34×10^{11}	2.37×10^{11}	2.47×10^{11}	2.72×10^{11}	3.00×10^{12}	4.82×10^{12}
2,5-OFQP	5.87×10^{10}	5.96×10^{10}	6.21×10^{10}	6.82×10^{10}	7.53×10^{10}	1.20×10^{11}
2,6-TFBP	1.78×10^{12}	1.80×10^{12}	1.89×10^{12}	2.09×10^{12}	2.34×10^{12}	4.14×10^{12}
2,6-HFTP	2.46×10^{12}	2.50×10^{12}	2.60×10^{12}	2.87×10^{12}	3.19×10^{12}	5.38×10^{12}
2,6-OFQP	2.01×10^{12}	2.05×10^{12}	2.14×10^{12}	2.37×10^{12}	2.65×10^{12}	4.68×10^{12}
			cc-pVTZ			
2,6-TFBP	1.96×10^{12}	1.99×10^{12}	2.08×10^{12}	2.31×10^{12}	2.58×10^{12}	4.56×10^{12}

SI Table 6. Marcus rate constants (Unit: s^{-1}) in hole transport for different values of $E_r^{\rm ex}$ (see SI Table 4).

Molecule	k_M ($E_r^{\rm ex}$ = 0 meV)	k_M ($E_r^{\rm ex}$ = 25 meV)	k_M ($E_r^{\rm ex}$ = 50 meV)
		6-31G(d)	
2,3-TFBP	2.77×10^{10}	2.12×10^{10}	1.63×10^{10}
2,3-HFTP	1.88×10^{8}	1.44×10^{8}	1.11×10^{8}
2,3-OFQP	1.26×10^{9}	9.61×10^{8}	7.36×10^{8}
2,5-TFBP	8.24×10^{11}	6.30×10^{11}	4.83×10^{11}
2,5-HFTP	9.66×10^{10}	7.39×10^{10}	5.66×10^{10}
2,5-OFQP	3.94×10^{9}	3.01×10^{9}	2.30×10^{9}
2,6-TFBP	1.08×10^{13}	8.23×10^{12}	6.31×10^{12}
2,6-HFTP	1.28×10^{13}	9.80×10^{12}	7.50×10^{12}
2,6-OFQP	1.05×10^{13}	8.01×10^{12}	6.14×10^{12}
		cc-pVTZ	
2,6-TFBP	6.15×10^{12}	4.72×10^{12}	3.62×10^{12}

SI Table 7. Marcus rate constants (Unit: s^{-1}) in electron transport for different values of $E_r^{\rm ex}$ (see SI Table 5).

Molecule	k_M ($E_r^{\rm ex}$ = 0 meV)	k_M ($E_r^{\rm ex}$ = 25 meV)	k_M ($E_r^{\rm ex}$ = 50 meV)
		6-31G(d)	
2,3-TFBP	4.11×10^{8}	3.17×10^{8}	2.45×10^{8}
2,3-HFTP	3.67×10^{6}	2.83×10^{6}	2.18×10^{6}
2,3-OFQP	6.38×10^{7}	4.91×10^{7}	3.79×10^{7}
2,5-TFBP	6.59×10^{10}	5.08×10^{10}	3.91×10^{10}
2,5-HFTP	2.59×10^{10}	2.00×10^{10}	1.54×10^{10}
2,5-OFQP	7.10×10^{9}	5.46×10^{9}	4.21×10^{9}
2,6-TFBP	1.60×10^{11}	1.23×10^{11}	9.52×10^{10}
2,6-HFTP	2.48×10^{11}	1.91×10^{11}	1.47×10^{11}
2,6-OFQP	2.32×10^{11}	1.79×10^{11}	1.38×10^{11}
		cc-pVTZ	
2,6-TFBP	1.76×10^{11}	1.36×10^{11}	9.75×10^{10}

2.4 Optimized Structures

SI Table 8. The atomic coordinates of the optimized 2,3-TFBP monomer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	9.1064037706946159	7.9992173858814555	3.1158847157616765
F	7.0398463798673507	9.6776437825954620	3.0843679345190353
C	8.2797496236313979	7.9712010127253725	2.0611912686413514
C	7.2069322075406790	8.8541545442592717	2.0394517330815582
C	6.3377358815186193	8.8934099652558487	0.9641674121881685
H	5.5090750704883718	9.5929969546397817	0.9751432874711368
C	6.5576468766781533	8.0271563819162992	-0.1051947061405585
H	5.8863292255587671	8.0448624830930466	-0.9569705786268715
C	7.6280876999103162	7.1405157389726295	-0.0841383943944196
H	7.7895411393760376	6.4600080331824854	-0.9140182490095924
C	8.5071275335793928	7.0945572378141781	1.0049855614518552
F	9.0684944712597861	5.2657836726772533	3.1158847635872315
F	11.1350517268023665	3.5873570567452293	3.0843678948057023
C	9.8951486169033736	5.2937999993147198	2.0611913227143845
C	10.9679659485368184	4.4108463609216546	2.0394517435690460
C	11.8371622705919979	4.3715909387369436	0.9641674180131915
H	12.6658230009731998	3.6720038305547082	0.9751432830501436
C	11.6172512697740924	5.2378444698736697	-0.1051947360935377
H	12.2885689238952551	5.2201382786545185	-0.9569706149175798
C	10.5468105563643366	6.1244852379388277	-0.0841383738796796
H	10.3853570892939420	6.8049928927902616	-0.9140182611711624
C	9.6677707167610585	6.1704437414562578	1.0049855753789068

SI Table 9. The atomic coordinates of the optimized 2,3-HFTP monomer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	9.1200386738798915	8.0102056148188279	3.1064112349939470
F	7.0439451919911766	9.6772087983523853	3.0740663612858103
C	8.2899526171952989	7.9731615132125686	2.0548791057686162
C	7.2123767329765025	8.8501119950920426	2.0324253000528256
C	6.3397849615003734	8.8792883025047225	0.9595541797638564
H	5.5069117453669945	9.5738969395485132	0.9700520692270562
C	6.5612166761919024	8.0096432090434764	-0.1067738219102611
H	5.8870740314802541	8.0198628852142999	-0.9564019125698267
C	7.6363735294958994	7.1287834973933153	-0.0853296743873812
H	7.7986095145726546	6.4449487241980297	-0.9123262759918217
C	8.5179860147788471	7.0925114791843944	1.0019612377207381
F	9.0933504491092361	5.2821613606012088	3.1256476283118730
F	11.1394950060313978	3.6102749639280782	3.1100110386946711
C	9.9186346226367696	5.3101087274520413	2.0712825605133367
C	10.9934624525015323	4.4321192309427522	2.0626386457686010
C	11.8771300299137366	4.3787134309566627	0.9899308362855821
C	11.6309756703092084	5.2309242684734611	-0.0919907422503426
H	12.3061245059024387	5.2118754043683033	-0.9413640470204723
C	10.5555991825520135	6.1084575516895780	-0.0835861783415476
H	10.3943241186994193	6.7740466734049578	-0.9252660461628852
C	9.6804045503964637	6.1722059283142734	1.0064097475973732
F	13.7857816727806224	4.2394438658397382	3.0827848185136610
F	15.8459383785303434	2.5543805828024491	3.0798517389579105
C	13.9248584431237603	3.4068679982408199	2.0417176814358702
C	15.0063522352248473	2.5353061488393931	2.0348360085008390
C	13.0193579022354182	3.4334614538016641	0.9854955474301034
C	15.2202293368228752	1.6742259433821411	0.9737940687084511
C	13.2415837750331953	2.5653948831825462	-0.0905071600360610
C	14.3276644150175478	1.6969333950903653	-0.0964513331979204
H	12.5439453187277579	2.5720790829363418	-0.9219980707371395
H	14.4810971837817366	1.0265178567214099	-0.9351662244947836
H	16.0747210612398668	1.0066182904692940	0.9949416775693158

SI Table 10. The atomic coordinates of the optimized structure of 2,3-OFQP monomer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	9.1053281318549555	8.0367623643830655	3.0994439638345979
F	7.0403234681782596	9.7169375886986042	3.0211788149771879
C	8.2910605003756697	7.9963773470705162	2.0357526654942966
C	7.2195101182163084	8.8798021039003050	1.9894272190471674
C	6.3634419140212408	8.9051140496327132	0.9032149054597296
H	5.5350703289184162	9.6049847864290570	0.8947701165451274
C	6.5952113142178481	8.0249842555017139	-0.1522603248756908
H	5.9341048522935278	8.0319128474144996	-1.0120435362450553
C	7.6644057625448285	7.1378533449223953	-0.1071515188068890
H	7.8349687756297275	6.4459645305972311	-0.9256577895817888
C	8.5293799345956263	7.1058087647375361	0.9936784095055542
F	9.0639902532599415	5.3071440971060166	3.1391383598623195
F	11.0893736604606996	3.6099795448578700	3.1559041632045224
C	9.9022480215263187	5.3203957586416495	2.0949567256815951
C	10.9665788582474484	4.4293714979606431	2.1038778213737968
C	11.8606154013673137	4.3587093803362453	1.0408634881318384
C	11.6389630209237396	5.2102486232235101	-0.0471532455579667
H	12.3238126267459478	5.1790432427373192	-0.8882231160349127
C	10.5742984948561887	6.1001139416651284	-0.0560422211303946
H	10.4308752940614173	6.7625716092264696	-0.9032723922425082
C	9.6854672687456507	6.1780413824382725	1.0219339825321021
F	13.7518579411693391	4.1447086373553752	3.1566084003193167
F	15.7782198508774414	2.4486860164873065	3.1449401604105542
C	13.8759168019016936	3.3232083372938099	2.1063726543200736
C	14.9408063891108487	2.4328129515977115	2.1001189251840708
C	12.9828001334143277	3.3913011299503215	1.0424335898321320
C	15.1590827134956694	1.5732995919467829	1.0289194884834310
C	13.2057886586201736	2.5376407650615542	-0.0436668011938893
C	14.2710030331552051	1.6484211077724928	-0.0498909331917613
H	12.5217291217857642	2.5668521278747445	-0.8854523687089330
H	14.4156460821802579	0.9844151893762444	-0.8957029498525833
F	15.7406725318909793	-0.2807552719754043	3.1103644791638616
F	17.8078886552764537	-1.9583663677254715	3.0362280904444678
C	16.5552898016547232	-0.2414182654013190	2.0469052288297469
C	17.6280568126046866	-1.1234926084048957	2.0027525768553400
C	16.3162446452495473	0.6468136540590737	1.0030204260650573
C	18.4846666375443824	-1.1497460214481758	0.9169943880059311
C	17.1817730796809549	0.6138034067619161	-0.0973466628283320
C	18.2521803663810864	-0.2719547051195409	-0.1402792383018953
H	17.0106927708586326	1.3039202356337167	-0.9172432740270992
H	18.9136995661289511	-0.2796059619766929	-0.9997368390781761
H	19.3140164059780801	-1.8484650106003284	0.9103241680940201

SI Table 11. The atomic coordinates of the optimized structure of 2,5-TFBP monomer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	1.2650699212500498	10.2977637803099800	13.2262488889386507
F	2.9968138918509180	6.2506891471044321	16.3874193856091104
F	3.5423258469579375	10.0605413269320874	11.7385221538617319
F	1.4141366857928785	5.7149390300577183	9.2988740789955262
C	1.7174453916900929	9.2997070819810315	14.0017955446166980
C	1.6067596183486976	9.4284351683447696	15.3770170761484337
H	1.1767277279269697	10.3324886783349292	15.7931131266764044
C	2.0420859666180577	8.3930030693928899	16.1970245006627636
H	1.9711999693488504	8.4607256271241731	17.2767261763876867
C	2.5724831853002019	7.2573304667105756	15.6049844452643285
C	2.6861053097166776	7.1270569356831617	14.2306562322228789
H	3.1195757729886582	6.2265518987387063	13.8088398546685394
C	2.2579568730836130	8.1644491963581025	13.3981817980624669
C	2.3489250420283403	8.0334289386431230	11.9240568775277218
C	2.9916342141514418	8.9920200562771662	11.1408411693612397
C	3.1064541047359437	8.8724520310446078	9.7651559892784849
H	3.6206692205981432	9.6464454751309496	9.2067656809635245
C	2.5694604524084155	7.7584209654143539	9.1291363039004843
H	2.6416497053211256	7.6323353252849522	8.0547271158493512
C	1.9364779008789037	6.7966329035720490	9.9011137218384295
C	1.8184060848618426	6.9149889115687859	11.2761232171498893
H	1.3017471141422825	6.1454939859913607	11.8396766620156768

SI Table 12. The atomic coordinates of the optimized structure of 2,5-HFTP monomer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	1.2895440952886474	10.3010233263367041	13.2139803412011592
F	2.9539916870182052	6.2421668008852356	16.3963098647883356
F	3.5746709195207922	10.0695615638794980	11.7521069612152704
F	1.4721112920555035	5.7265795151356187	9.2941008119400248
C	1.7259817799390058	9.3003928483689542	13.9958101672245849
C	1.5921313765203704	9.4268844953301869	15.3690811226194395
H	1.1581589627567543	10.3313418107843216	15.7800546243975948
C	2.0101865529053882	8.3881752658915616	16.1939493569294548
H	1.9210087101239877	8.4540564317815612	17.2723808460260067
C	2.5467349937154315	7.2517867358522761	15.6086156030274736
C	2.6837247761248455	7.1234865611286651	14.2363305224355692
H	3.1208978925089066	6.2223119967127829	13.8198714122154449
C	2.2732982750884205	8.1645891114426163	13.3993714389951517
C	2.3886090059530689	8.0369194463115221	11.9275174066496756
C	3.0349701192202581	8.9978555707405388	11.1516327022837896
C	3.1714210839789816	8.8766107094992819	9.7802499179787823
H	3.7002007100103027	9.6476822883319056	9.2304425321307502
C	2.6584099270494970	7.7591072450102008	9.1186661895522647
C	2.0119840259045461	6.7982325820417140	9.8945200016013466
C	1.8755274083854276	6.9194794150881060	11.2659337855028294
H	1.3466916968688141	6.1484044406300802	11.8156774322428966
F	2.0930737194928599	9.5530012513997082	4.6494340359112831
H	1.9260642482134998	9.5734086968314305	7.2259743740863556
C	2.5004559242509461	8.5436596463082815	5.4374119445512274
C	2.3633187800856934	8.6722096104673305	6.8096470454978739
C	3.0372962161572024	7.4072492649721386	4.8523593102658342
C	2.7738302709357350	7.6313108501828948	7.6468160120501096
C	3.4555149386052859	6.3687828924476868	5.6774316828495248
C	3.3214593828237997	6.4954997276672746	7.0506724637438385
H	3.8897120274205768	5.4643565380711321	5.2666304812608775
F	3.7581587753360761	5.4951625780006603	7.8327278965356104
H	3.1266004257412021	7.3412307824681102	3.7739417122894459

SI Table 13. The atomic coordinates of the optimized structure of 2,5-OFQP monomer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	1.2521353367402086	10.3637500647005840	13.1552794855114641
F	2.8826133582851559	6.3357843487313374	16.3877942489005939
F	3.5358797177034660	10.1115697004564815	11.7151129463605503
F	1.4801739630233037	5.7294837409764767	9.2868984721251699
C	1.6760066448600142	9.3673794148784815	13.9485807711294516
C	1.5226442760783410	9.5064325561662262	15.3163071128378903
H	1.0771044787644783	10.4129021780613247	15.7116346904789559
C	1.9139419589372542	8.4769982452022532	16.1749320779964734
C	2.4595805273385478	7.3327029543836817	15.5950192182060476
C	2.6133893140966991	7.1934902019956093	14.2272128095989707
H	3.0587451675522401	6.2869066329974954	13.8318888630335426
C	2.2218318687163898	8.2231490785834378	13.3689302920415649
C	2.3560368766005215	8.0763078200849030	11.9013058076585097
C	3.0074781965135355	9.0301457450207607	11.1209521049721811
C	3.1599870562282919	8.8932558313220618	9.7528360304034223
H	3.6907142237645054	9.6602185329670895	9.1991560977357416
C	2.6588235277854833	7.7653599829251139	9.0998726937474981
C	2.0085150418417186	6.8109661298318649	9.8806750111195552
C	1.8556534294174112	6.9476797205706733	11.2487428244100354
H	1.3239646544154984	6.1811960486724242	11.8021884265644914
F	2.1223454724223902	9.5021761145747181	4.6047622068814551
H	1.9364711483965746	9.5542365945389562	7.1801517166099771
C	2.5282710652658089	8.5041864463883385	5.4085685993780013
C	2.3798525218819280	8.6496318984618643	6.7778889829778883
C	3.0740805666043070	7.3629929313016627	4.8413724826205993
C	2.7883444383077052	7.6206462114529065	7.6307440244298910
C	3.4907679621154242	6.3366325386018270	5.6823560072751826
C	3.3455126531272525	6.4801737459413156	7.0527581782248232
H	3.9313898706352695	5.4291851955221171	5.2852214615484536
F	3.7802104908741954	5.4911743942116171	7.8511678885488498
F	2.6286331401160403	10.9748001122339947	20.2682213612615314
C	2.1251559094930319	9.8857763471308466	19.6621342459212798
H	2.8214244593264683	10.5147351563027751	17.7368616330154296
C	2.2875417147277748	9.7518078630849168	18.2932996766011158
C	1.4670133758691863	8.9338203033014949	20.4254587730351602
C	1.7772377601451208	8.6249898566016849	17.6430646615559361
C	0.9495085615882239	7.8122484137330028	19.7864813798441617
C	1.1087846970030926	7.6764238136107918	18.4168276095529571
H	0.4165696711954720	7.0461627432743894	20.3381997341467056
F	0.5749973449545261	6.6015190702839268	17.8134308110485193
H	3.1719051768941671	7.2835260765873331	3.7645653560124233
H	1.3597423803930400	9.0729352443312656	21.4953232246772963

SI Table 14. The atomic coordinates of the optimized structure of 2,6-TFBP monomer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	1.8215691877001130	4.5783477618096260	13.2913616501044434
F	-0.2612747576701216	6.1652832516331530	17.1976288684249390
F	-0.0363111551547742	8.7166074157372702	11.7291773597352176
F	1.9967617466706389	10.1163446588104406	15.7118108131748357
C	0.7847388968011613	5.4531394181219639	15.2136186364013550
C	1.4124856314841436	7.8568857459728623	15.4712105351634523
C	1.2649242715404330	4.3564316235007494	14.4943626147432667
C	0.1477448396146942	3.8701640309250891	16.9719552641697717
C	0.2302395429057714	5.1547894403615562	16.4602038166652207
C	0.8559487372669602	6.8406131777073380	14.6892196111689106
C	0.4400320360902308	8.4373235621064211	12.9532461232713914
C	0.3631439135349907	7.1332073937885463	13.4141588078123970
C	1.2096015760073129	3.0530327245765192	14.9603899802048801
C	0.6443675832893041	2.8171362640514706	16.2099632418949753
C	1.4605736103458318	9.1427920773219018	14.9582632938334630
C	0.9832307575767854	9.4715650311833759	13.6992498506566971
H	-0.3013929569259312	3.7117438848273472	17.9457103257831001
H	1.8077592124686694	7.6587200358240048	16.4603004993751760
H	1.6064755296229580	2.2499308402501015	14.3502834035925577
H	-0.0793645133208199	6.3674989346775357	12.7880256228175053
H	1.0316608084146857	10.4842027523376569	13.3169793323490424
H	0.5907055017369727	1.8039899744751109	16.5940503486574222

SI Table 15. The atomic coordinates of the optimized structure of 2,6-HFTP monomer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	1.7549469651994651	4.6202337111844249	13.2511334709661881
F	-0.1941410605195778	6.1738089514808481	17.2394754030661908
F	-0.0811486821023987	8.7624981525743273	11.7738232325081675
F	2.0015811966272778	10.1262937139629994	15.7611026278095121
C	0.7849078970585477	5.4790647060236441	15.2152332017076724
C	1.4075728358249937	7.8837915865682833	15.4886070948391854
C	1.2341531733389040	4.3875593691200399	14.4680369900324628
C	0.1902587681286063	3.8790036169045976	16.9729475262955951
C	0.2669312885802711	5.1692133417935278	16.4749764834753130
C	0.8494766750931495	6.8709799232147288	14.7056176773018663
C	0.4195971781279901	8.4881211642217167	12.9893928607899980
C	0.3492563848979197	7.1819971933651665	13.4392856207821172
C	1.1828440354541436	3.0790652800226668	14.9195361056835463
C	0.6544701258739595	2.8318293778158101	16.1829513479558535
C	1.4490091207606446	9.1739580736640285	14.9920455093277099
C	0.9648575498717233	9.5352053123376219	13.7338664989384114
H	-0.2303019802481191	3.7114633470682281	17.9579129669533728
H	1.8182011545302841	7.6825244569325806	16.4706812476044213
H	1.5532328593642193	2.2808011047092589	14.2867335995435791
H	-0.1028653251670103	6.4281758115777876	12.8058639740293270
H	0.6040863558792218	1.8142939739199537	16.5558029206802040
F	2.1438700332385725	12.7487160013150493	10.3089086916617187
H	1.9580210366647546	10.3936743966655705	11.3390663099482936
C	1.6178107503580188	12.4992500315514832	11.5188190928061616
C	1.5715914374341133	11.1888071212689315	11.9653537894462243
C	1.1486732580416994	13.5686896411636724	12.2653858346053308
C	1.0271592582230236	10.9282030763089804	13.2262947822830608
C	0.6171166614128430	13.2703981248350047	13.5101921289506155
C	0.5436481287903551	11.9802796848124284	14.0094095906416065
F	0.1496928949237372	14.2790816893689101	14.2629778070378688
H	0.1110005672389547	11.8069941270457850	14.9875822936731193
H	1.1946094570997241	14.5852939372018771	11.8937133186551698

SI Table 16. The atomic coordinates of the optimized structure of 2,6-OFQF monomer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	1.8001067885120914	4.6163722930526507	13.2790022239094263
F	-0.2470814719242184	6.1952692331817527	17.2077530056194981
F	-0.0044574777900962	8.7541803264819986	11.7361134273627314
F	1.9694720340465346	10.1400703893858708	15.7708816140191779
C	0.7820418098277224	5.4873896493446255	15.2131166618379581
C	1.3922379061361709	7.8941311847928084	15.4907383335427991
C	1.2499181190558213	4.3913646574749263	14.4843097479868685
C	0.1451769323832262	3.8989859127412991	16.9666228002098620
C	0.2333015621124661	5.1857538824759262	16.4618609271771348
C	0.8578998707307895	6.8764762840965785	14.6973833476808835
C	0.4664767221857006	8.4856056762799597	12.9646517405066426
C	0.3902320093575807	7.1807888993904507	13.4170207359823426
C	1.1883705380187903	3.0859788380291144	14.9434526013633437
C	0.6295395826541470	2.8469942937617385	16.1953576777149806
C	1.4409147337712020	9.1827636316349182	14.9914207355336426
C	0.9868214223541145	9.5377429219462471	13.7201045070100900
H	-0.2990872523154631	3.7379845728656691	17.9422588206104408
H	1.7773202791681175	7.6974701026003425	16.4840480310596931
H	1.5751542429992662	2.2834475858109071	14.3260268795208923
H	-0.0420668495236042	6.4231120332645286	12.7744098712282224
H	0.5711363166646212	1.8319931224318076	16.5739491682857789
F	2.1904470029464176	12.7365125593196851	10.3024206247610781
H	2.0009936445873668	10.4086968461057143	11.3310608704569908
F	2.3418759015221098	18.2597411450435310	12.7824303215589961
C	1.6443064417926125	12.5044609044845245	11.5069650497117735
C	1.6002704544410487	11.1972058161020200	11.9566285216530535
C	1.8121642706684222	17.2889681500634609	12.0210506234481862
C	1.3294706344622196	17.6254489613004317	10.7660864842591497
C	1.7758031480943630	15.9980621922922559	12.5222313700581509
H	2.1752795665828346	15.7937385135138921	13.5083971459417516
C	0.7932593846079906	16.5939958835196428	10.0112574989562386
C	1.2265194966128963	14.9850874178706484	11.7309156946655548
C	1.1689983937901338	13.5925093407772941	12.2407410959263157
C	0.7285672102109315	15.2848586218200229	10.4595487693029217
F	0.3119324810583959	16.8808273593258420	8.7910804986288724
C	1.0504084516323011	10.9294227013031939	13.2120968685852134
H	0.2912175908793383	14.5215333956523178	9.8269713317086858
C	0.6321245031432438	13.2728000445096779	13.4888460377358506
C	0.5606815960078937	11.9839637265552099	13.9855569143933334
F	0.1402979156679846	14.2663821300996645	14.2465325878173896
H	0.1153776255190982	11.8168096979282531	14.9589976609185875
H	1.3688464673474041	18.6419991013687465	10.3933811713494002

SI Table 17. The atomic coordinates of the optimized structure of 2,3-TFBP dimer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	9.2207074099601254	7.8492942223405819	3.2348339728048354
F	7.3744093317838448	9.7564427438055770	3.3301871450573333
C	8.4428547977164516	8.0336309211744563	2.1596223471537992
C	7.4841493490373150	9.0377284558646096	2.2029905519280129
C	6.6675418923467804	9.2913444688081501	1.1165753983550140
H	5.9240949041285598	10.0780911109973417	1.1804223439151602
C	6.8264096893912258	8.5189938955319793	-0.0330877883004659
H	6.1888395124200022	8.7039139026419079	-0.8910374159766875
C	7.7830765975109060	7.5108250323080803	-0.0786951703938706
H	7.8943509656555380	6.9035605847735955	-0.9715996089386347
C	8.6048767800281869	7.2466686241058733	1.0234150316722535
F	8.7771133793459448	5.1740264996018634	2.9489541543478777
F	10.6115136277339417	3.2423529705388154	2.8665438394966944
C	9.6716367982869151	5.1860438845668702	1.9514462603717939
C	10.6214306018829916	4.1730740327883433	1.9021467214840999
C	11.5512138018924642	4.1187095405622705	0.8792227233115163
H	12.2848381838835294	3.3198085444890229	0.8669934017456041
C	11.5171095870431124	5.0998461903968479	-0.1103061873882525
H	12.2416646555818964	5.0701689893452260	-0.9170975481868680
C	10.5686942158354888	6.1156735015235828	-0.0624511579719731
H	10.5505205907293167	6.8830441926197841	-0.8300778351976916
C	9.6327924242097573	6.1786231927086126	0.9768836071495607
F	6.1351049038540202	12.0096876453875030	4.6524179371831691
F	4.2175675214077133	10.1654226112798423	4.7436736355322182
C	5.3281681571093813	11.8778580613619322	3.5929646416425496
C	4.3311273270516857	10.9113572136337336	3.6368242148121999
C	3.4774555604684982	10.7217978911449681	2.5656645466556425
H	2.7066266389264975	9.9615632391480524	2.6305946665045790
C	3.6419144062639046	11.5127886660469922	1.4287127994172832
H	2.9769331529213567	11.3740818259323735	0.5832933512412685
C	4.6437886907941976	12.4766649146413116	1.3801783883734577
H	4.7662727179049176	13.0951818692877850	0.4967498316635702
C	5.5031900296205452	12.6756501834845796	2.4674663014221676
F	5.7493270602057391	14.7465905015958132	4.3751262915225588
F	7.6577800604489923	16.6057382343337139	4.2922601307741095
C	6.6522448147510946	14.6908188451240616	3.3865500378530826
C	7.6420015291947889	15.6642084553749310	3.3386175568902230
C	8.5861787254333812	15.6682183132055588	2.3272654248628792
H	9.3491586080445259	16.4391277112658436	2.3130954692814205
C	8.5259889795841595	14.6761906173947985	1.3498468439778737
H	9.2628832293515906	14.6639385912870353	0.5537600428950558
C	7.5357229653992155	13.7001985488015716	1.3955229823304527
H	7.4950781079117741	12.9233946792711745	0.6380319916564716
C	6.5821177169476099	13.6926558795034783	2.4203581270685981

SI Table 18. The atomic coordinates of the optimized structure of 2,3-HFTP dimer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	9.3803905715999818	7.8157919563101208	3.3248991185963224
F	7.4979874809046319	9.6762467499794855	3.4326348087069096
C	8.6275012805817788	8.0167867870685274	2.2353990597732407
C	7.6485346535884551	9.0005151640864813	2.2849414647610047
C	6.8568935352631621	9.2774241769474948	1.1855101351248278
H	6.0995935327610322	10.0517224365808691	1.2530002817877222
C	7.0613094855914573	8.5445999152006493	0.0168706952702829
H	6.4457724602010842	8.7456269943198777	-0.8533885593754680
C	8.0364430003941720	7.5540901846135453	-0.0345123332743163
H	8.1808317033128493	6.9782468884991280	-0.9432948703133198
C	8.8343431450794512	7.2693332112941942	1.0801598155235315
F	9.0279875228940423	5.1699482696642702	2.9778599263815368
F	10.8910456886895339	3.2932149830727258	2.9099483477954999
C	9.9385570891278636	5.2233716312974341	1.9979802697912752
C	10.9150402242478481	4.2377222656442903	1.9614188972103670
C	11.8770664038225231	4.2106779940605676	0.9569864593621642
C	11.8119665281320554	5.2012779887449980	-0.0287662875485119
H	12.5555348451969575	5.2054428661154599	-0.8192776327533946
C	10.8355632619707372	6.1875853969520760	0.0080062153665662
H	10.8153830257949242	6.9582055770570932	-0.7559389741502818
C	9.8834969429430224	6.2234286098168292	1.0325780494788002
H	12.5122867175110528	2.5705626678268692	-1.1037238246640946
H	14.2988894740447137	0.8515015652624386	-1.1784979165357716
C	13.1438963655905958	2.4000366999836245	-0.2374506000891645
C	14.1433559923289582	1.4339680192859210	-0.2765879818863763
C	12.9203696053745229	3.1578748666538621	0.9188232586227436
C	14.9464533602348375	1.2031748834279463	0.8391802699839085
C	13.7362315893418199	2.9237864068058599	2.0210066761167580
C	14.7320014649052506	1.9556326072204657	1.9801840449488184
F	13.5902510674053545	3.6415059502282157	3.1427703274601888
F	15.4862746738290742	1.7719304582284323	3.0726078766842342
H	15.7291770881070150	0.4522873275657409	0.8356021854766291
F	6.4354668248757605	11.8370063104369638	4.6933071047650881
F	4.5756468197629454	9.9375512317853296	4.7798236088196360
C	5.5251017674475547	11.7955064226053778	3.7140040830945273
C	4.5549205986387982	10.8011039021591486	3.7560370493462694
C	3.5977986787538998	10.6964275482354676	2.7634381613855505
H	2.8499990621434867	9.9135009756390904	2.8280055932102126
C	3.6240487938771899	11.6086170585757689	1.7089212148016142
H	2.8742364316002793	11.5434629228462136	0.9280278665831576
C	4.5994043657569694	12.5976186800186767	1.6587927517352425
H	4.6100360800465880	13.3127776281232606	0.8424697271421188
C	5.5696895280870979	12.7067942113742234	2.6634314273509587
F	6.2060499214881819	14.5068589877966332	4.7843984802415331
F	8.0723799983510549	16.3670792518968540	4.6111199137891532
C	6.9012613892060539	14.5915309201439136	3.6436785516168491
C	7.8784453686571778	15.5727459972493367	3.5507467485104387
C	8.6202030378181540	15.7504258935255539	2.3872806669272912
C	8.3350335260717188	14.9106552726129902	1.3058627428700464
H	9.0090074964561500	15.0243122619291825	0.3867364741297004
C	7.3618544060221440	13.9254416821350091	1.4007626402726299
H	7.1720782747175269	13.2666303598564923	0.5594410661177218
C	6.6285779732276673	13.7400239809874716	2.5793803500098904
F	12.6477599461723447	17.8030831619617942	4.1059269028743328
F	10.7433327257582558	15.9433289212525882	4.2367014227689435
C	11.6866878228756494	17.8072712638427753	3.1720087787634230
C	10.6888415901489946	16.8439927582880955	3.2462685086762080
C	11.6936485182676719	18.7462846153015370	2.1560076297839372
C	9.6664502235393250	16.7975049975814734	2.3036620202414793
C	10.6816453265432383	18.7052940942960042	1.1982242916120500
C	9.6810478040945931	17.7417781158018997	1.2700753280973891
H	10.6724481041902113	19.4374424056594108	0.3977442804616814
H	8.8911287807240118	17.7172879137077608	0.5257583395972550
H	12.4814957807191735	19.4910687525574815	2.1220270707710154

SI Table 19. The atomic coordinates of the optimized structure of 2,3-OFQP dimer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

C	8.7500187886862566	8.1578592616371086	2.2591825040203224
C	7.7852300924734976	9.1568474459155897	2.2937754597580908
C	7.0133286763425096	9.4399903235549072	1.1823764343823067
H	6.2648109466433128	10.2221133360408789	1.2376620604143693
C	7.2224389464761209	8.7049687591085299	0.0165734903341141
H	6.6214255062812395	8.9147798340312843	-0.8617923384964502
C	8.1843303967905090	7.7019396304225118	-0.0206465642497664
H	8.3345019316386626	7.1230787183587791	-0.9265423570438930
C	8.9608390791035859	7.4070170613544706	1.1063936688827891
F	9.1045998883458115	5.2974588234394204	2.9999458560414536
F	10.9183290569983011	3.3715717028206442	2.9178313853988622
C	10.0191922659037722	5.3353359580017141	2.0234005353318918
C	10.9690577667454079	4.3242799610614462	1.9789928167345727
C	11.9311619109570870	4.2803711603324510	0.9751491782960646
C	11.8967919948590666	5.2821848270724878	-0.0008367337045312
H	12.6425276449899524	5.2743242982591196	-0.7892629770111892
C	10.9461379597087287	6.2926642717437673	0.0432743903832866
H	10.9479111965615150	7.0695177541028000	-0.7145621475815925
C	9.9921652660996063	6.3435726570810829	1.0654478143221930
H	12.5662364363026704	2.6641785409982890	-1.1142904430388274
H	14.2841865649899340	0.8896668379140634	-1.1852038138037002
C	13.1714573706556077	2.4607134283219096	-0.2366415376261236
C	14.1364670380371127	1.4632051413759923	-0.2757284898412788
C	12.9435611357286824	3.1996408412444861	0.9299249713987130
C	14.9126253084803739	1.1634043541470400	0.8489360448824342
C	13.7299563233080804	2.9104341609875650	2.0396076485742873
C	14.6950566803866778	1.9141218170620791	1.9998689902595106
F	13.5956281156272798	3.6096071182523670	3.1729983240524144
F	15.4338397572813832	1.7116522565479235	3.0974758783085452
F	15.0507775003312414	-0.9362746781469443	2.7457409424488253
F	16.9078855287590670	-2.8473649982199909	2.6874240270296244
C	16.9332560645969110	-1.9038906429513776	1.7360823680962139
C	15.9716993594183396	-0.9017030537763923	1.7734112309266044
C	17.8906329997282008	-1.9339670203508150	0.7378015956766802
C	15.9493322833812616	0.1045921168535566	0.8122045524148396
C	16.9132330302744514	0.0662989017343002	-0.2025746992906082
H	16.9095649084293278	0.8442308038083031	-0.9596986448485544
C	17.8726820879345603	-0.9396110356515857	-0.2388046417085890
H	18.6186934284477772	-0.9498223930719101	-1.0262562054241728
H	18.6326209007097994	-2.7252328729973025	0.7346713312121591
F	6.2384523456341832	12.0559069614249594	4.7280404986551625
F	4.3381141657742708	10.1906482256661430	4.7513934964429065
C	5.4774554689367498	11.9086210021009418	3.6376041084123272
C	4.4890683542758083	10.9320475207081440	3.6461436585585085
C	3.6826949403250202	10.7268786571457166	2.5413691531857565
H	2.9177932168452694	9.9587997640786661	2.5780532583165501
C	3.8827235283892736	11.5154086806178402	1.4085880407748119
H	3.2571257011981212	11.3645993813339850	0.5354982869319582
C	4.8756876429287255	12.4894846539163016	1.3949518142546067
H	5.0289830176036219	13.1032164179436030	0.5129698997482440
C	5.6893762018700942	12.7011950256615478	2.5149335966029951
F	5.9222696325013331	14.7666157182229369	4.4425847795831590
F	7.8254757976896263	16.6067335012029851	4.4035462946575628
C	6.8422990583241647	14.7012099081220331	3.4723562334855957
C	7.8418477691624799	15.6639140559593688	3.4535574436659773
C	8.8172599177402340	15.6719417942010519	2.4611029508937463
C	8.7452858967839955	14.6843346343893160	1.4726937386561596
H	9.5003583011486565	14.6636814185875473	0.6934417442629712
C	7.7435135846462435	13.7231077163815289	1.4901905229569228
H	7.7148807932417274	12.9537731887971610	0.7250062638154670
C	6.7727407305487768	13.7125372397997882	2.4973347488597204
F	12.4054381308664219	18.0995257117817587	4.6160225017503480
F	10.5097344704317326	16.2555105834348907	4.6694861447794889
C	11.6646052942550540	17.9279173132521912	3.5145021264843943
C	10.6686130865105948	16.9615006107989501	3.5435209777602528
C	11.9077322917827093	18.6826393365143382	2.3715069990698963
C	9.8732148634569263	16.7113072995472898	2.4306945467837253
C	11.1254557710074451	18.4179492895393970	1.2420761412554679
C	10.1289003221312601	17.4517503982064603	1.2708932646814302
H	11.2929694752453091	18.9955517216094982	0.3386326139994953
H	9.5190505901757536	17.2758669145551700	0.3905254609347095
F	13.9787460079057695	22.6347448094248875	4.2504489327761830
F	12.0850721794969065	20.7605907484935592	4.2868251378948674
C	13.9910217027458934	21.6971352087474756	3.2930721504417289
C	13.0094729060766561	20.7141935353851920	3.3182687603293557
C	14.9540930156928464	21.7149704407457165	2.3000131921947125
C	12.9705914215471481	19.7159915929168470	2.3492587580302162
C	14.9218968636100229	20.7270799350176311	1.3171961264807450
C	13.9419392369579391	19.7405859525890186	1.3410035328003311
H	15.6724569647291450	20.7267841796667653	0.5339722915909700
H	13.9266758710812244	18.9676810724063039	0.5788889880086462
H	15.7105151556625291	22.4924411768683790	2.3055984987642204

SI Table 20. The atomic coordinates of the optimized structure of 2,5-TFBP dimer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	5.9155226031111994	2.4075221148503632	6.4051542940683790
F	4.1391571252821153	6.7034335686698219	3.6205833685174542
F	3.7964093123859532	2.6423350177309599	8.1064727300457662
F	6.1822428359764192	6.8530640978748174	10.5472798723124317
C	5.4587365628785829	3.4693033387386305	5.7227510477396279
C	5.4568278577602713	3.4137464535835882	4.3378680991164851
H	5.8065365098006385	2.5143243342912798	3.8442200676013676
C	5.0077807626795448	4.5104098064615030	3.6105285765158883
H	4.9820794459935778	4.4973933894021600	2.5268761606669936
C	4.5808914008573769	5.6302556729254407	4.3056544554806528
C	4.5786427953526099	5.6888539776613420	5.6875310498174345
H	4.2062428655374253	6.5780303915336473	6.1849216860010152
C	5.0220572708909010	4.5902388745268290	6.4270900308963963
C	5.0303465408057653	4.6504688759985964	7.9076725525943230
C	4.4090660188560538	3.6841106322553689	8.6980184339622379
C	4.3709012743706399	3.7634864172085742	10.0807284508306054
H	3.8651165125115452	2.9866666763964393	10.6430110346817948
C	4.9730731691235990	4.8421203694950217	10.7195207226018336
H	4.9653692431774568	4.9311343053006587	11.7998260693170032
C	5.5940259622327382	5.8080969208968902	9.9432106333884001
C	5.6298191044655201	5.7315897649831316	8.5608820518551170
H	6.1366103302544568	6.5042195110589942	7.9926971809826339
F	2.3976019310799819	2.1784379816446640	3.3178802573848314
F	0.6005231641928698	6.1620803270896447	6.5194683140468674
F	0.0367028397766476	2.5285010406553714	1.8131205092038531
F	2.5642700312200990	6.7009423472348306	-0.5462909221442799
C	1.9206638096890816	3.1555990245415355	4.1062236983824878
C	1.9911569330739534	2.9952912445795046	5.4793381882375360
H	2.4195048801692507	2.0893855490397466	5.8906078898729195
C	1.5356574118764472	4.0138600959792408	6.3084258141376068
H	1.5832625042203434	3.9261236482969903	7.3872240485113814
C	1.0316267468348088	5.1656833949151544	5.7263322409202653
C	0.9611187873323834	5.3288813577546952	4.3522966788188233
H	0.5549351972846067	6.2449532440312376	3.9375522734945787
C	1.4059620495178113	4.3064727972117165	3.5119785933762331
C	1.3701859596655384	4.4587755941239733	2.0376334520256592
C	0.6711828087020119	3.5598892472190999	1.2331078833086784
C	0.5958681445078905	3.6978725420349434	-0.1432964021772332
H	0.0288007433083587	2.9787595595688257	-0.7231627839593994
C	1.2358833307000245	4.7710067195613144	-0.7560463481328806
H	1.2019588083365413	4.9061159262040794	-1.8311754142292178
C	1.9359926645013779	5.6661921094156016	0.0373183170233181
C	2.0093624958089666	5.5333520526776248	1.4145315041341771
H	2.5860932538966042	6.2392596843762460	2.0004236387700005

SI Table 21. The atomic coordinates of the optimized structure of 2,5-HFTP dimer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	5.9976380932679687	2.4731511012311387	6.4256102855477089
F	4.1711823523439460	6.6853492738347446	3.5462565670687995
F	3.9024258318266325	2.6708097406872433	8.1293845834007730
F	6.0782714996655915	7.0496890222079562	10.4571920743157296
C	5.5230913373597801	3.5114261909816227	5.7196796444893865
C	5.5339842192262516	3.4306557708287682	4.3359730622527941
H	5.9071506344619289	2.5301835347884829	3.8618623224147925
C	5.0724936778931484	4.5054438402218313	3.5840648455912083
H	5.0586916944423468	4.4740939321183975	2.5005784128181343
C	4.6184325516607272	5.6297448543695632	4.2545054831340776
C	4.5975752440914066	5.7114615851593076	5.6347206636737264
H	4.2032138041776106	6.6019700427152941	6.1123420807903095
C	5.0548564652522199	4.6351900677485736	6.3987723943886214
C	5.0442979756933832	4.7273281970394381	7.8767590040002444
C	4.4594899648107340	3.7586454439569517	8.6906029002281269
C	4.3830653403232347	3.8866209303781298	10.0665445303518517
H	3.8835051816629642	3.1156863395783363	10.6433533448022342
C	4.9115351118701449	5.0145653614294909	10.6968034408919248
C	5.5187392894955467	5.9727900670149330	9.8869050829229899
C	5.5854595615294453	5.8488465705378410	8.5112593997171011
H	6.0771530613657783	6.6239889015791045	7.9334629409921709
C	4.8302810722875931	5.1697166868939046	12.1678218785929708
C	4.2728781050184486	6.3108122793454395	12.7455759370153885
F	3.8094369150889253	7.2841045115751450	11.9458544963771551
C	4.1577383995049697	6.4684878499157490	14.1171911859030530
H	3.7171408277741862	7.3765105875547086	14.5128738481068638
C	4.6049665977748058	5.4579887422365836	14.9614529051262011
H	4.5347787508533948	5.5463556930105744	16.0396457847386777
C	5.1521544649744779	4.3167110739368031	14.3949417148074730
F	5.5876642439766080	3.3340028065903691	15.2003025757322803
C	5.2699259855965694	4.1569618695972599	13.0239010299935902
H	5.7125552261121255	3.2514598890588884	12.6227830417221547
F	2.4614211519731661	2.1482120089759067	3.3401031446633205
F	0.6340895265186959	6.0693978378576015	6.6015796898675116
F	0.0871077862252835	2.4565163979050508	1.8607695686776073
F	2.4435932343842537	6.7405787396671091	-0.4664360570918638
C	1.9781576518359472	3.1095122289056247	4.1442622085260776
C	2.0673037844554134	2.9376465637819456	5.5150039280656600
H	2.5129900623175128	2.0344464434821092	5.9137872531942550
C	1.6021247615380820	3.9396933170167818	6.3590310761188080
H	1.6593265945548696	3.8416840017236558	7.4364126943465463
C	1.0733667647561560	5.0887563976403651	5.7938487858506109
C	0.9833268743819974	5.2635461010319009	4.4225437109864272
H	0.5562877968582738	6.1757630679352697	4.0203750637253339
C	1.4348182217931300	4.2560905558876589	3.5674279739031522
C	1.3661574599551547	4.4220808373446907	2.0963548852104719
C	0.6789908370649312	3.5170293386788862	1.2899796131748353
C	0.5591813530943018	3.6831636851423664	-0.0787345585125022
H	-0.0131366695189350	2.9665177405828129	-0.6574679839130335
C	1.1383820910665363	4.7916863399829897	-0.7006234573940948
C	1.8400820387510333	5.6865046969365372	0.1044569573398713
C	1.9547799540234012	5.5242172739468112	1.4735929770285785
H	2.5301435399492713	6.2358080719851845	2.0531575788769376
C	1.0257788411458950	4.9855220681986516	-2.1657729637382186
C	0.4976474311142912	6.1593379090766973	-2.7028636536810766
F	0.0836363624437337	7.1262979289935870	-1.8686830216688362
C	0.3629674094985031	6.3569796234105702	-4.0675627257317082
H	-0.0546477901435483	7.2883130866290777	-4.4327459923305739
C	0.7636236685894096	5.3554104417978481	-4.9455413871029297
H	0.6780345190801046	5.4748073792903007	-6.0197678191744846
C	1.2819475437573944	4.1822244331198668	-4.4193634444044383
F	1.6734615712569858	3.2086935254518569	-5.2582823791560092
C	1.4177466563031931	3.9821127621535193	-3.0550537479000681
H	1.8379154895923486	3.0534564373442161	-2.6840253796642251

SI Table 22. The atomic coordinates of the optimized structure of 2,5-OFQP dimer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	6.1126769922440767	2.3762602014211711	6.4332786169187353
F	4.3704037211294446	6.5729347787451573	3.4792619793010764
F	4.0237218196404907	2.6619517021520838	8.1408058421556788
F	6.3082875084158214	7.0328527541985579	10.3764999821023256
C	5.6582355369281165	3.4115203773872915	5.7089592495132653
C	5.6591590960437772	3.3031161672721980	4.3271129912902992
H	6.0103603498503704	2.3859369917780784	3.8684636065472899
C	5.2187344487328016	4.3732861668869445	3.5560093607576269
H	5.2010257943166005	4.3220497687922590	2.4733346480585974
C	4.7946691586809678	5.5206281384976430	4.2068090130389564
C	4.7838612552701676	5.6301078675676903	5.5853335752370237
H	4.4143838295399513	6.5391314125704847	6.0476221923362585
C	5.2210420644938491	4.5589771852366718	6.3685840260556237
C	5.2186799650024360	4.6817410849769017	7.8447276511185091
C	4.6044303576190373	3.7492492709881313	8.6789844630637560
C	4.5204394033176207	3.9136823261262421	10.0504408129631333
H	3.9900376535784918	3.1760455128343033	10.6428730583471776
C	5.0751493574644133	5.0430164518029086	10.6553141224166747
C	5.7201738494688739	5.9597447797347396	9.8268294873823194
C	5.7904429186607453	5.8017457652280715	8.4549864373694188
H	6.3097239213121128	6.5456044085649374	7.8605982777261003
C	4.9799535286310297	5.2448138400524096	12.1189806190586538
C	4.4759115965403478	6.4284504645482352	12.6561632374967434
F	4.0694042983180507	7.4005945375273150	11.8255538267981315
C	4.3472966472317784	6.6302235937148239	14.0187588491883020
H	3.9363732713879402	7.5656358668910153	14.3827580559165149
C	4.7197019809644916	5.6261704285990497	14.9139944656807639
C	5.2194228243824270	4.4410348565435056	14.3773605496501897
F	5.6120703075121909	3.4649256438445559	15.2100776231630590
C	5.3527450570218882	4.2403163629152134	13.0146597378800912
H	5.7630263024389858	3.3043587512007369	12.6511070134691348
C	4.6063361901777329	5.8340525197163737	16.3771825931301649
C	5.2134724804219807	6.9347508812448639	16.9872059318503474
H	5.8103520224092833	7.6254494248446782	16.4017767819528899
C	5.0709899908646650	7.1232415748727043	18.3522671419968688
F	5.6691200109472977	8.1817034606998504	18.9246685554959093
C	4.3328086536457411	6.2583817227158924	19.1454091990395554
H	4.2473756348520455	6.4371096647565977	20.2114968665659305
C	3.7200881481708064	5.1627370019571472	18.5453101601050356
H	3.1241596005821592	4.4683403791050216	19.1262165746866977
C	3.8633001631662398	4.9701511335817372	17.1806123720210486
F	3.2495116972802971	3.9209223040481094	16.6091839800684227
F	2.5294213960216907	2.0904877330470941	3.3594890918309721
F	0.8168770228557718	6.0428737334501239	6.6467116563228439
F	0.1269605098047862	2.4287108793791399	1.9256696115597522
F	2.4852503560312731	6.6851038448686495	-0.4511762545098394
C	2.0755329945759087	3.0603030749477935	4.1712919755137525
C	2.1891773678461632	2.8904018865201015	5.5404309546155979
H	2.6304365629069473	1.9823630468671563	5.9331842641066332
C	1.7526670280927530	3.9002320682623060	6.3907351061885045
H	1.8291468087330356	3.8022467532745701	7.4668654543787394
C	1.2289531440296051	5.0549673394854748	5.8328623297459785
C	1.1144834182233987	5.2281435432985806	4.4632414639983704
H	0.6912659607983693	6.1446913218113455	4.0667897319076722
C	1.5357303385678724	4.2122547234959002	3.6024469940351644
C	1.4376009114929684	4.3766606134969006	2.1329552512570804
C	0.7193875633653918	3.4822274003979912	1.3418418732053501
C	0.5678723456666122	3.6527380540411638	-0.0230860208390669
H	-0.0273535490035540	2.9454552003850694	-0.5900678009611871
C	1.1462787160094334	4.7556997344712366	-0.6560064350367126
C	1.8813486684939040	5.6381533014690657	0.1330760407898698
C	2.0274717454601410	5.4711746232667942	1.4984304200634735
H	2.6252115505340679	6.1729608192162875	2.0670414646728954
C	0.9941404870747964	4.9576254184642989	-2.1155501284173450
C	0.4988846002050675	6.1519413944690102	-2.6361622453842828
F	0.1476596347140412	7.1349737797183597	-1.7929565553639282
C	0.3263109330974466	6.3549067468576377	-3.9936286259305449
H	-0.0754104860767591	7.2991294758419514	-4.3450379613179537
C	0.6477253944351619	5.3431182387788390	-4.9002006582696849
C	1.1391418485494336	4.1474254667813204	-4.3797572678075349
F	1.4884490139016013	3.1640201540908337	-5.2234175670917073
C	1.3130093230796320	3.9444734027661532	-3.0217022856260711
H	1.7152864855044274	3.0003313376773924	-2.6704680400866740
C	0.4997338105088417	5.5607296295726094	-6.3589343289880196
C	-0.2672768522376033	4.7102439525030677	-7.1543641337368484
F	-0.8805103681904960	3.6622988464775483	-6.5801274364934166
C	-0.4363994767837168	4.9163458023400057	-8.5143363441213697
H	-1.0479312716575224	4.2309862050761788	-9.0897465145416891
C	0.1726476013726733	6.0123094365681462	-9.1175541426889861
H	0.0670903047579065	6.2013083461406255	-10.1801161446821808
C	0.9324681682879348	6.8651696288593840	-8.3319391735144617
F	1.5263704841651891	7.9246726665156855	-8.9069262366537512
C	1.1022108011932501	6.6623867298731856	-6.9722636747117068
H	1.7148192949347638	7.3439761190328374	-6.3924712363312004

SI Table 23. The atomic coordinates of the optimized structure of 2,6-TFBP dimer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	5.5481870263450377	4.4083732115718508	13.4252684156723348
F	3.4563272723097507	6.1008899182871916	17.2864324592094327
F	3.5013499522392784	8.3964432038501631	11.7097496678382154
F	5.5106455730709092	10.0743062083926791	15.5959225031494899
C	4.5125364033824633	5.3403122700615899	15.3202734254596091
C	5.0399725468595111	7.7794085661566079	15.4615600690293640
C	5.0172198307314009	4.2260741717178991	14.6466105237086612
C	3.9552696959775715	3.8191646892891966	17.1588456641104372
C	3.9824952507501896	5.0785691911965891	16.5860108488112594
C	4.5312975925000547	6.7023496210237532	14.7314740344941395
C	4.0226993914150064	8.1950251922357662	12.9315598836277790
C	4.0225549573472135	6.9110316803897645	13.4470609540017669
C	5.0142993614735456	2.9446533626287881	15.1731058429747243
C	4.4780284089626736	2.7488453772468060	16.4415508448299228
C	5.0212831061264982	9.0415237787127989	14.8910026308221450
C	4.5220492485457804	9.2879468822950493	13.6220393036828380
H	3.5206685780225326	3.6951600046934256	18.1437304913006372
H	5.4441845067489822	7.6522273272795758	16.4588452720675953
H	5.4313933353081456	2.1275331408462557	14.5955568892049801
H	3.5917791012950855	6.1010910211920892	12.8738315021883540
H	4.5059213505865516	10.2857892834993443	13.2015547590091558
H	4.4636426175946466	1.7527501639794572	16.8701486224774939
F	1.6708302234754173	4.7735572633533341	13.0363749355816392
F	0.0072617038078735	6.1652237175806626	17.2199529920750614
F	-0.0389396215237020	8.9796531593601419	11.7699922447792940
F	1.9860239484032931	10.2178572002825181	15.8088203194920656
C	0.8466072072143981	5.5699295675002372	15.1012181327873822
C	1.4085732767592190	7.9711412542497735	15.4760721931718859
C	1.2487411995308859	4.5068994719574187	14.2870508655551713
C	0.4012804369886491	3.8938427728518707	16.8391355439756616
C	0.4258561251076727	5.2008365742322775	16.3826278928435158
C	0.8681643546821423	6.9826547332745088	14.6469026114459240
C	0.4331096753869695	8.6535345134943000	12.9839684649111913
C	0.3715399055023096	7.3297429446346376	13.3873888087302788
C	1.2521874006899458	3.1845409634342778	14.6960545631425017
C	0.8206017245995607	2.8819096938112070	15.9821965496170648
C	1.4421943537746413	9.2760622789237992	15.0195082199318026
C	0.9592413658326517	9.6593483141782599	13.7781578242914371
H	0.0531146298066925	3.6874265585079327	17.8447620290488018
H	1.8356099860957482	7.7284178033759545	16.4396406925289469
H	1.5875243907547330	2.4183689377381596	14.0066037510540635
H	-0.0537097154112650	6.5893443490643442	12.7209059978214984
H	1.0025373921044278	10.6865339257349934	13.4373322132029536
H	0.8184849288248524	1.8532057359128922	16.3255385463417824

SI Table 24. The atomic coordinates of the optimized structure of 2,6-HFTP dimer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	5.4629468247107296	4.4321018644538865	13.3465156318525278
F	3.5063546988115339	6.0566595342811169	17.3063953911692252
F	3.5752848253263618	8.5155168363818134	11.7808458185154183
F	5.6382004086039501	10.0000157757038739	15.7432633765554773
C	4.5010862863886532	5.3316024248328269	15.2953051874699995
C	5.0790260699368126	7.7486841451313628	15.5121046882295666
C	4.9654419061758306	4.2270692077797358	14.5779258111117844
C	3.9734660749463155	3.7729145534163648	17.1117929031598663
C	4.0015889358086500	5.0451223742685487	16.5688411964503182
C	4.5454415720439805	6.7089036714268424	14.7494528548829589
C	4.0974345089439588	8.2822593474024622	12.9986968216858259
C	4.0526091835125841	6.9853534585084223	13.4734525672575920
C	4.9576121055980060	2.9333825975848637	15.0730118505663153
C	4.4582432116750850	2.7136926000083110	16.3522397289714370
C	5.1035946833498240	9.0272512815333368	14.9871770912349636
C	4.6248550494385050	9.3580044845845478	13.7174820484929061
H	3.5615074611046564	3.6296275228963291	18.1038014002433663
H	5.4843306398859966	7.5811448806793846	16.5027036921765600
H	5.3397721183644506	2.1254796923994421	14.4594811960216560
H	3.5916189821120335	6.2175465716161780	12.8663503481513644
F	5.5461836829404794	12.5286009263522864	10.1733808128664567
H	5.4495444620350932	10.1938578315614592	11.2413698336947334
C	5.1115421722527685	10.9920346852706405	11.8911996339072825
C	5.1164233758274209	12.2960411172665154	11.4240647142401421
C	4.6600149034125273	10.7432754493219829	13.1903335367554284
C	4.7010738234337062	13.3743672652178347	12.1882689579108536
C	4.2570627672988683	13.0866852558141940	13.4695031250034489
C	4.2313875472033766	11.8057388397565433	13.9908610619053331
H	3.8458600771598728	11.6471477115031163	14.9889088426259711
F	3.8158476957540639	14.0986683038285836	14.2345803797706907
H	4.4413350467978274	1.7079769661982052	16.7576158436957989
H	4.7022970505568473	14.3843438209439647	11.7974927453025025
F	1.7469925941055493	4.6398441404341684	13.1205208579703925
F	-0.0062064780888497	6.1360845321633573	17.2285472368035109
F	-0.0246860488313945	8.7491207277489753	11.6992572956363485
F	1.9731045290061231	10.1488147989006450	15.7238265449886025
C	0.8658578393491809	5.4824341846958271	15.1413408985723397
C	1.4146397052493851	7.9041739080715532	15.4392943721895701
C	1.2771322854698486	4.3989108796439647	14.3593119498743551
C	0.3627135971974600	3.8502425617544116	16.9023167666299265
C	0.4147599514800706	5.1477220807043702	16.4213296128247173
C	0.8934000300345748	6.8793437400575179	14.6467598273145683
C	0.4621134675866199	8.4907816433152945	12.9237487818371743
C	0.4094463347700742	7.1848963188918882	13.3736676010328051
C	1.2461371605700240	3.0846763951016376	14.7910610031818468
C	0.7796226264377745	2.8150352965770784	16.0727187040818507
C	1.4407662370522660	9.1925925624389819	14.9413019968954881
C	0.9760591211237162	9.5506665367484675	13.6735930572143705
H	-0.0078756213684355	3.6703056145237554	17.9049685370746161
H	1.8384553950083689	7.7077174643946709	16.4150417332088026
H	1.5880950112625436	2.3003294126719305	14.1258125480816776
H	-0.0129870606916429	6.4249982128820591	12.7275103660420932
F	2.0700851660466730	12.7283227082586823	10.1959072098918231
H	1.9034702850787117	10.3900371999575665	11.2504445759957736
C	1.5226509573797595	11.1876398399190844	11.8748943328330849
C	1.5648506663837700	12.4927263616245874	11.4181284963655241
C	1.0211023422070109	10.9391168490671280	13.1557111298762024
C	1.1276325229506627	13.5727708559270450	12.1690621169547271
C	0.6442811019433555	13.2873078935269096	13.4358264850865030
C	0.5789263328171305	12.0018031722861078	13.9476946546012943
H	0.1825405706935440	11.8455012770756163	14.9436316264184406
F	0.2194933421071345	14.3052741279219475	14.2015834580108393
H	0.7544810927881934	1.7930867516357516	16.4347893601537294
H	1.1719867914698592	14.5861809531539226	11.7895377704792601

SI Table 25. The atomic coordinates of the optimized structure of 2,6-OFQP dimer molecule using ωB97XD functional and 6-31G(d) basis set. The unit of atomic position is in Å.

F	3.6655086310787302	8.5031150159263866	11.7640522038132858
F	5.5857549693799466	10.0244544687458834	15.7820167722737068
C	4.4820363797916576	5.3481579488256337	15.3339070110094298
C	5.0439170708902763	7.7686111767261270	15.5501055863035393
C	4.9635706509535753	4.2378718688313057	14.6368269031107552
C	3.9152560036923254	3.8045517676320588	17.1513875701324245
C	3.9549367197725314	5.0721326975795682	16.5988354673593541
C	4.5390985169718459	6.7211824338577388	14.7781981229260726
C	4.1437473678115353	8.2792464885463453	13.0013275210501327
C	4.0876931032166386	6.9860273252645095	13.4840921681833485
C	4.9471453070326525	2.9486072752264660	15.1430951012601973
C	4.4189650765975230	2.7395831564635658	16.4125794431749554
C	5.0800949390366270	9.0434346265405221	15.0173593168694843
C	4.6423277505323020	9.3619120409275496	13.7300060928274181
H	3.4830594681725340	3.6693531828433588	18.1358733334197595
H	5.4196788054293163	7.6107597875582433	16.5537656828345661
H	5.3460379686487691	2.1355952924920083	14.5472608088710107
H	3.6549862296376534	6.2108323536587049	12.8656782638956635
F	5.7216364282983907	12.4675563507388407	10.1927890085333246
F	3.8912496569334700	16.5737292181294684	8.6339218019353279
H	5.5541962897483836	10.1753313984668701	11.2749442095237580
H	3.9254182638598047	14.2444265214524144	9.7222508502227143
C	5.1927403132008667	10.9774402835220926	11.9069043631517548
C	5.2297094357705944	12.2739993602581308	11.4272335202320647
C	4.3621325798388355	15.0257537838375814	10.3297124450689743
C	4.3933147261248298	16.3245621825465044	9.8546435785310926
C	4.9059199566260263	17.3856644977589561	10.5847306653075854
C	4.6983714503986214	10.7400558248775404	13.1906337324956802
C	4.8560306426748898	14.7650241807013725	11.6108491459689027
C	4.8075020250029024	13.3870549043054101	12.1562524853983955
C	5.3879240855651265	17.0878212956608451	11.8492322410374076
C	5.3796490650729680	15.8081823979224492	12.3793235305294846
C	4.3216074401137545	13.0936035807195648	13.4328074967473032
C	4.2578827366630048	11.8185058774963423	13.9597051017654668
H	5.7765309624422123	15.6412273185689514	13.3733962562491602
F	5.8885145268067252	18.0876505801704859	12.5927717447581404
H	3.8350430384438963	11.6823184348881632	14.9462032401702452
F	3.8623672962321329	14.1015236631946816	14.1957855961481023
H	4.3948341163421363	1.7372800143264400	16.8259327158092660
H	4.9115185062745308	18.3958613688961776	10.1945651035233880
F	1.8429964860499430	4.5748477103031870	13.1620549948664181
F	-0.1274490765980757	6.0997539384072921	17.1577407559510853
F	0.0738671054470675	8.6896173601735320	11.6461617333408221
F	1.9637149848237823	10.0885061048759006	15.7223270268136339
C	0.8503045247609904	5.4278559022594832	15.1241463216458367
C	1.3994027683588099	7.8457657233382339	15.4291152249013397
C	1.3080137587965450	4.3401319795655917	14.3751910999450185
C	0.2701176799401194	3.8119000988817948	16.8746774982900192
C	0.3376364445812088	5.1048091060913432	16.3835301039133867
C	0.8986919042994540	6.8216921212964650	14.6223758187064856
C	0.5238873261142688	8.4307961883291149	12.8842885416078303
C	0.4576139281461987	7.1250245946541124	13.3334062917913698
C	1.2631804953645509	3.0299139776123578	14.8180200021301740
C	0.7343437070711072	2.7712691390420341	16.0777413695930242
C	1.4458576683848663	9.1325211048227786	14.9299409077310408
C	1.0153602953001934	9.4902722206583476	13.6500320691798205
H	-0.1459631044396611	3.6397843540504646	17.8606422197551318
H	1.7910913585326416	7.6492196894671327	16.4180816877842908
H	1.6473631856514870	2.2404911423693603	14.1825009514847409
H	0.0569552311281068	6.3638466186028610	12.6746188919649061
F	0.3441198258744715	16.8335028994263780	8.7057167270911915
F	2.0957482953188378	12.6729711652646078	10.1863613321894597
H	0.3207670807943647	14.4779491360455470	9.7421387645218722
H	1.9431220563793474	10.3644766594697799	11.2248970048110888
C	0.7377545698773001	15.2434611819777786	10.3855496650179528
C	0.8024273105789624	16.5518927792964412	9.9358305434991312
C	1.5604419986369080	11.1491476734784616	11.8643798733897068
C	1.5959537365723639	12.4553629558683099	11.4162596779827599
C	1.0672557039395281	10.8805350762663604	13.1426040573602183
C	1.1714454923887023	13.5518935437936374	12.1703223286455042
C	1.2155269252275926	14.9450642009715491	11.6645645669691813
C	1.3184976451420327	17.5869086628429763	10.6989348846201420
C	0.6972796178268605	13.2294188443263234	13.4439474312362037
C	0.6346832741740990	11.9406570523029494	13.9406858416232105
C	1.7879496952421574	17.2496536859216434	11.9588366528521437
C	1.7473921512461748	15.9620368799705226	12.4627837155278929
H	0.2357446426441351	11.7833039292299375	14.9353025019088097
F	0.2573873360150192	14.2217146655653366	14.2344659848373212
H	2.1588401663964429	15.7583483378016886	13.4421763927182614
F	2.3233197852530569	18.2191025144106042	12.7192279556155707
H	0.6990977615021099	1.7528601534533201	16.4489381588160661
H	1.3640876253917011	18.6017764247864825	10.3235087370504601

3 SI References

[1] Malpass, J. R.; Hemmings, D. A.; Wallis, A. L.; Fletcher, S. R.; Patel, S. *J. Chem. Soc., Perkin Transactions 1* **2001**, 1044–1050.
[2] Chołuj, A.; Kula, P.; Dąbrowski, R.; Tykarska, M.; Jaroszewicz, L. *J. Mat. Chem. C* **2014**, *2*, 891–900.
[3] Tsukada, S.; Kondo, M.; Sato, H.; Gunji, T. *Polyhedron* **2016**, *117*, 265–272.
[4] Coe, J. W.; Wirtz, M. C.; Bashore, C. G.; Candler, J. *Org. Letts.* **2004**, *6*, 1589–1592.
[5] Qiu, D.; Jin, L.; Zheng, Z.; Meng, H.; Mo, F.; Wang, X.; Zhang, Y.; Wang, J. *J. Org. chem.* **2012**, *78*, 1923–1933.
[6] Molander, G. A.; Biolatto, B. *J. Org. Chem.* **2003**, *68*, 4302–4314.
[7] `http://www.chem.wisc.edu/areas/reich/handouts/nmr/f-data.htm`.
[8] Roesner, S.; Buchwald, S. L. *Angew. Chem. Int. Ed. Engl.* **2016**, *55*, 10463–10467.
[9] Gray, G. W.; Hird, M.; Lacey, D.; Toyne, K. J. *J. Chem. Soc. Perkin Transactions 2* **1989**, 2041–2053.
[10] Glendenning, M. E.; Goodby, J. W.; Hird, M.; Toyne, K. J. *J. Chem. Soc. Perkin Transactions 2* **1999**, 481–492.
[11] Huang, Q.; Zhang, X.; Qiu, L.; Wu, J.; Xiao, H.; Zhang, X.; Lin, S. *Adv. Synthesis and Catalysis* **2015**, *357*, 3753–3757.
[12] APEX II, 2005, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
[13] SAINT Version 6.45A, 2003, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
[14] Sheldrick, G. M. *Acta Cryst. Sec. C: Structural Chemistry* **2015**, *71*, 3–8.
[15] SHELXTL V6.12, 2002, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
[16] Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A.; Puschmann, H. *J. Appl. Cryst.* **2009**, *42*, 339–341.