# Supporting Information

## Pyromellitic Dithioimides: Thionation Improves Air-Stability and Electron Mobility of *N*-Type Organic Field-Effect Transistors

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**Contents**

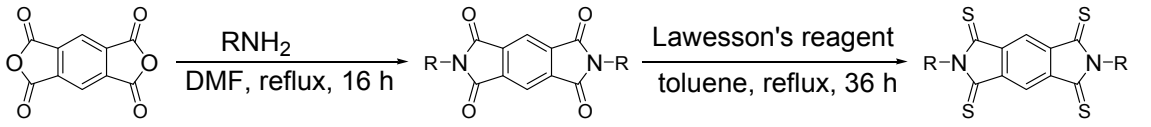
## 1. General information

Reactions were carried out in round bottom flasks fitted with rubber septa under argon. Crude product solutions were dried on $Na_2SO_4$ and concentrated with a rotary evaporator below 40 $^oC$ at ~30 Torr. Silica gel column chromatography was performed employing 230-400 mesh silica gel. Proton nuclear magnetic resonance ($^1H$ NMR) and carbon nuclear magnetic resonance ($^{13}C$ NMR) spectra were obtained using Bruker Avance II (300 MHz) NMR spectrometer. Chemical shifts (δ scale) are expressed in parts per million downfield from tetramethylsilane (δ = 0.00). $^1H$ NMR data are presented as follows: chemical shift, multiplicity (s = singlet, br = broad singlet, d = doublet, t = triplet, m = multiplet and/or multiple resonances), coupling constant in Hz (Hertz), integration. The molecular order of PyDTIs films were determined by X-ray diffraction (XRD, Rigaku 18 kW Rotating Anode X-ray Generator) using Cu Kα radiation ($\lambda_{K\alpha1}$ = 1.54 Å). Atomic force microscope (AFM) images were obtained using Veeco Dimension 5000 scanning probe microscope. Melting points were recorded with a Fargo (MP-1D) apparatus. High-resolution mass spectra were determined on a Jeol JMS-HX 110 spectrometer. Electrochemistry was performed using a CHI 760 electrochemical work station. Cyclic voltammetry was conducted using a three-electrode cell in which a BAS glassy carbon electrode (area: 0.07 $cm^2$) was the working electrode. The working electrode was polished with 0.05 μm alumina on Buehler felt pads. The auxiliary compartment contained a platinum wire separated by a medium-porosity glass frit. All cell potentials were taken using a Ag/AgCl, KCl (sat.) reference electrode.

## 2. Synthesis details

The PyDTI derivatives were synthesized using the methodology outlined in Scheme S1. The imidization reaction of pyromellitic dianhydride with different amines in the presence of dimethylformamide (DMF) gave PyDIs, which were then thionated with Lawesson's reagent in toluene to obtain PyDTI analogues.

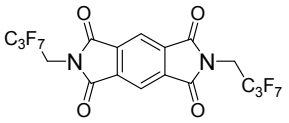
**Scheme S1.** Synthetic routes, reagents and conditions to PyDTI derivatives.




**PyDI-C8**: R = *n*-octyl
**PyDI-F**: R = $CH_2C_3F_7$

**PyDTI-C8**: R = *n*-octyl
**PyDTI-F**: R = $CH_2C_3F_7$

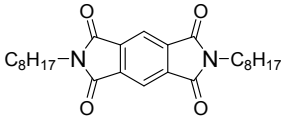
**Synthesis of N, N'-Di(2,2,3,3,4,4,4-heptafluorobutyl)pyromellitic diimide**[S1]



**PyDI-F**

To a stirred solution of pyromellitic dianhydride (2 g, 9.2 mmol) in anhydrous DMF (100 mL) was added 2,2,3,3,4,4,4-heptafluorobutylamine (3.6 g, 18.4 mmol). The reaction mixture was stirred at reflux for 16 h, then cooled to room temperature. The mixture was poured onto ice water and the precipitate was filtered. Purification by silica gel flash column chromatography (DCM) to give **PyDI-F** (2.6 g, 48%) as white solid. Mp: 232-233 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 8.46 (s, 2H), 4.44 (t, $^3J$ (H,F) = 15.3 Hz, 4H); $^{19}$F NMR (400 MHz, $CDCl_3$): δ -81.97, -118.23, -128.55; $^{13}$C NMR (75 MHz, $CDCl_3$): δ 164.6, 137.2, 119.9, 37.9, 37.6.

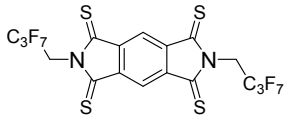
**Synthesis of N, N'-Di(*n*-octyl)pyromellitic diimide**[S2]



**PyDI-C8**

To a stirred solution of pyromellitic dianhydride (2 g, 9.2 mmol) in anhydrous DMF (120 mL) was added *n*-octylamine (2.6 g, 20.1 mmol), The reaction mixture was stirred at reflux for 16 h, then cooled to room temperature. The mixture was poured onto ice water and the precipitate was filtered. Purification by silica gel flash column chromatography (DCM-MeOH 10:1) to give **PyDI-C8** (3.0 g, 76%) as white solid. Mp: 189-190 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 8.24 (s, 2H), 3.17 (t, $J$ = 7.2 Hz, 4H), 1.68 (m, 4H), 1.27 (m, 20H), 0.85 (s, 6H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 166.4, 137.3, 118.2, 38.8, 31.8, 29.2, 28.5, 26.9, 22.7, 14.1.

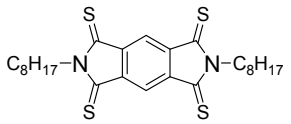
**Synthesis of N, N'-Di(2,2,3,3,4,4,4-heptafluorobutyl)pyromellitic dithioimide**



**PyDTI-F**

To a stirred solution of **PyDI-F** (0.12 g, 0.2 mmol) in anhydrous toluene (50 mL) was added Lawesson's reagent (1.1 g, 2.8 mmol),[S3] and the resulting mixture was stirred at reflux for 36 h. Then cooled to room temperature and concentrated in *vacuo*. Purification by silica gel flash column chromatography (DCM-hex 1:5) to give **PyDTI-F** (0.04 g, 30%) as dark brown solid. Mp:195-196 $^{o}$C. $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.47 (s, 2H), 5.28 (t, $^{3}J$ (H,F) = 15.3 Hz, 4H); $^{19}$F NMR (400 MHz, $CDCl_3$): δ -81.85, -114.53, -129.03 (m, 4F); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 194.8, 137.8, 120.5, 42.3; HRMS calcd for $C_{18}H_6F_{14}N_2S_4$: 643.9190, found 643.9197.

**Synthesis of N, N'-Di(*n*-octyl)pyromellitic dithioimide**



**PyDTI-C8**

To a stirred solution **PyDI-C8** (0.5 g, 1.1 mmol) in anhydrous toluene (100 mL) was added Lawesson's reagent (3.7 g, 9.1 mmol), and the resulting mixture was stirred at reflux for 36 h. Then cooled to room temperature and concentrated in *vacuo*. Purification by silica gel flash column chromatography (DCM-hex 1:3) to give **PyDTI-C8** (0.36 g, 63%) as dark brown solid. Mp: 110-111 $^{o}$C. $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.21 (s, 2H), 4.42 (t, $J$ = 7.8 Hz, 4H), 1.72 (m, 4H), 1.31 (m, 20H), 0.88 (s, 6H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 194.7, 137.4, 118.6, 44.7, 31.9, 29.2, 27.8, 27.0, 22.7, 14.2. HRMS calcd for $C_{26}H_{36}N_2S_4$: 504.1761, found 504.1771.

## 3. Single crystal structure

Single crystals of PyDTI-C8 were successfully grown by the slow diffusion of a poor solvent, hexane, into the PyDTI-C8 solution in $CHCl_3$. The solution of PyDTI-C8/$CHCl_3$ was put into the bottom of a clean test tube. Carefully layer the hexane onto the surface of

the solution and cover it with the aluminum foil. Then level the test tube under ambient conditions for one week. The single crystal data was summarized in Table S1. Single-crystal X-ray diffraction was performed on a Bruker APEX DUO at 100(2) K. Data were collected and processed by using APEX II 4K CCD detector.

**Table S1**. The crystal structure datum of PyDTI-C8 and PyDI-C14.

| | PyDTI-F (This work) | PyDI-C14 (Ref. 10) |
|---|---|---|
| Formula | $C_{26}H_{36}N_2S_4$ | $C_{38}H_{60}N_2O_4$ |
| M.W. | 504.81 | 608.88 |
| Temp. (K) | 100(2) | 150(2) |
| Wavelength | 0.71073 Å | 0.71073 Å |
| Crystal system | Triclinic | Monoclinic |
| Space group | P -1 | P $2_1$/c |
| Z | 1 | 2 |
| Lattice constants | | |
| *a* [Å] | 4.5302(2) | 38.939(3) |
| *b* [Å] | 10.3934(5) | 4.9902(3) |
| *c* [Å] | 14.1186(6) | 8.9040(5) |
| *α* [°] | 81.405(2) | 90.00 |
| *β* [°] | 86.591(2)° | 95.896(2) |
| *γ* [°] | 82.721(2) | 90.00 |
| V (Å$^3$) | 651.44(3) | 1721.01(19) |
| R-factor (%) | 3.39 | 5.94 |

## 4. Device fabrication and evaluation

### 4.1 Materials

Octadecyltrichlorosilane (ODTS, 95%, purchased from Acros), cyclic olefin copolymers (COC, purchased from Polyscience), and anhydrous toluene (Acros) were used as received. OFET devices were made using heavily n-doped Si substrates with 300 nm of thermally oxidized $SiO_2$ (capacitance $C_i$ = 10 nFcm$^{-2}$). The substrates were successively cleaned with deionized (DI) water, piranha solution ($H_2SO_4$:$H_2O_2$ = 7:3), DI water and finally blown dry with $N_2$ gas. ODTS-modified $SiO_2$ substrates were finally cleaned using PDC-32G plasma cleaner (Harrick) at low power for 1 min.

### 4.2 COC- and OTDS-modified substrates

The substrates modified by ODTS were prepared by immersing them into a 5 mM solution of ODTS in dry toluene for 6 hrs at preparing temperatures of 30 °C, controlled using a refrigerated circulator. Subsequently, the substrates were cleaned by ultrasonication in toluene and dried in flowing pure nitrogen. For the COC-modified substrates, 0.8 wt% solution of COC in dry toluene were spin-coated at 5000 rpm for 60 s. Finally, the modified substrates were baked at 120 °C in an oven for 1 hr to remove the residual toluene.

### 4.3 OFET Device Fabrication

Thin films (45 nm) of PyDI-F and PyDTIs were thermally evaporated onto the substrates at a rate of 0.1-0.2 $Å s^{-1}$ under a pressure of $5\times10^{-6}$ torr. The substrates were maintained at constant temperature of 25 and 50 °C, respectively. Finally, Au source-drain electrodes (40 nm) were thermally evaporated onto the thin films of organic semiconductors (top contact) through a shadow mask. The channel length ($L$) and width ($W$) are 100 μm and 2000 μm, respectively. All of the transistors were characterized under ambient air using Agilent Technologies B1500A Semiconductor Device Analyzer. The charge mobility ($\mu$) was calculated from the saturation regime using the formula, $I_d=(WC_i/2L)\mu(V_g - V_{th})^2$, where $L$ is the channel length; $W$ is the channel width; $C_i$ is the capacitance per unit area of $SiO_2$, $I_d$ is the drain current, $V_g$ is the gate voltage, and $V_{th}$ is the threshold voltage. The capacitance of COC-modified substrate obtained from metal–insulator–metal device is 4.05 $nFcm^{-2}$.

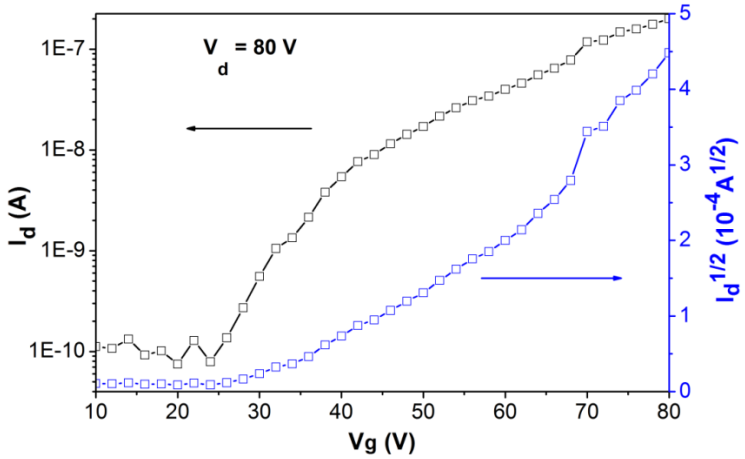


**Figure S1. Transfer characteristic of PyDTI-C8 device on COC-modified substrate ($T_s$ = 25 °C).**

## 5. X-ray diffraction and NMR spectra

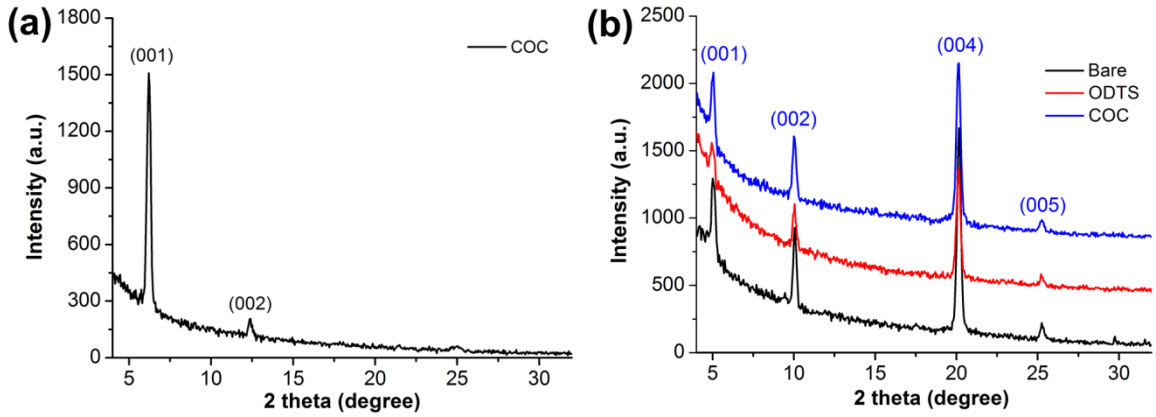



**Figure S2. XRD patterns of PyDTI films based on different substrates at $T_s$ = 25 °C (a) PyDTI-C8 and (b) PyDTI-F.**

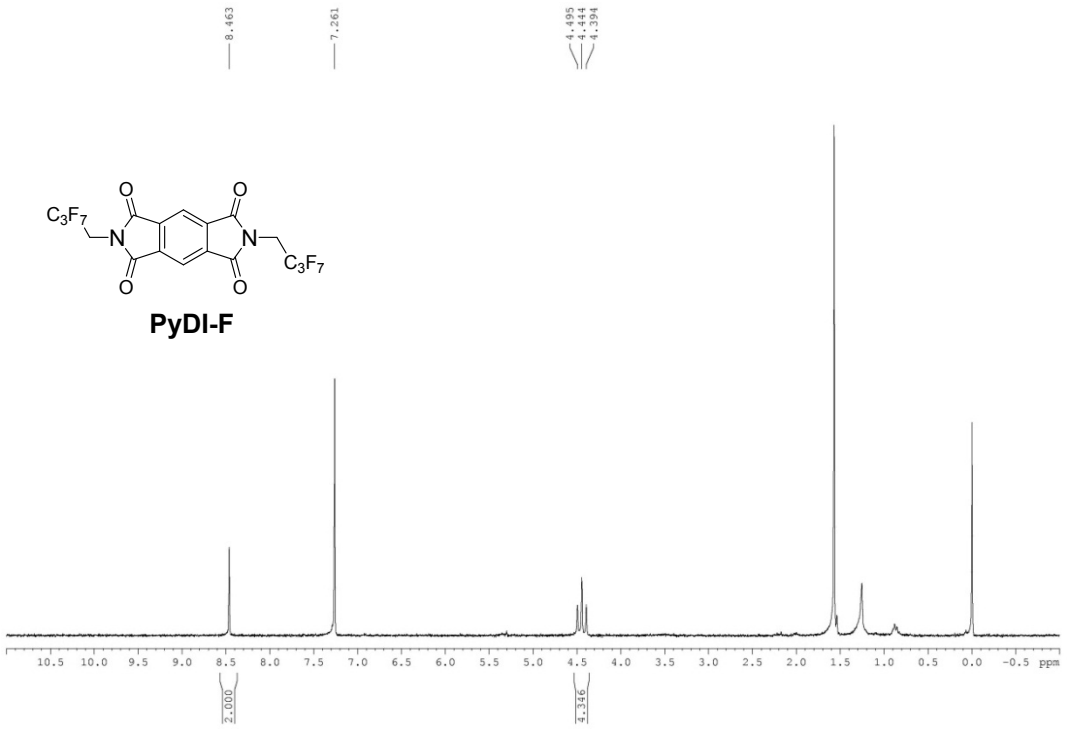



**Figure S3. $^1$H NMR spectra of PyDI-F.**

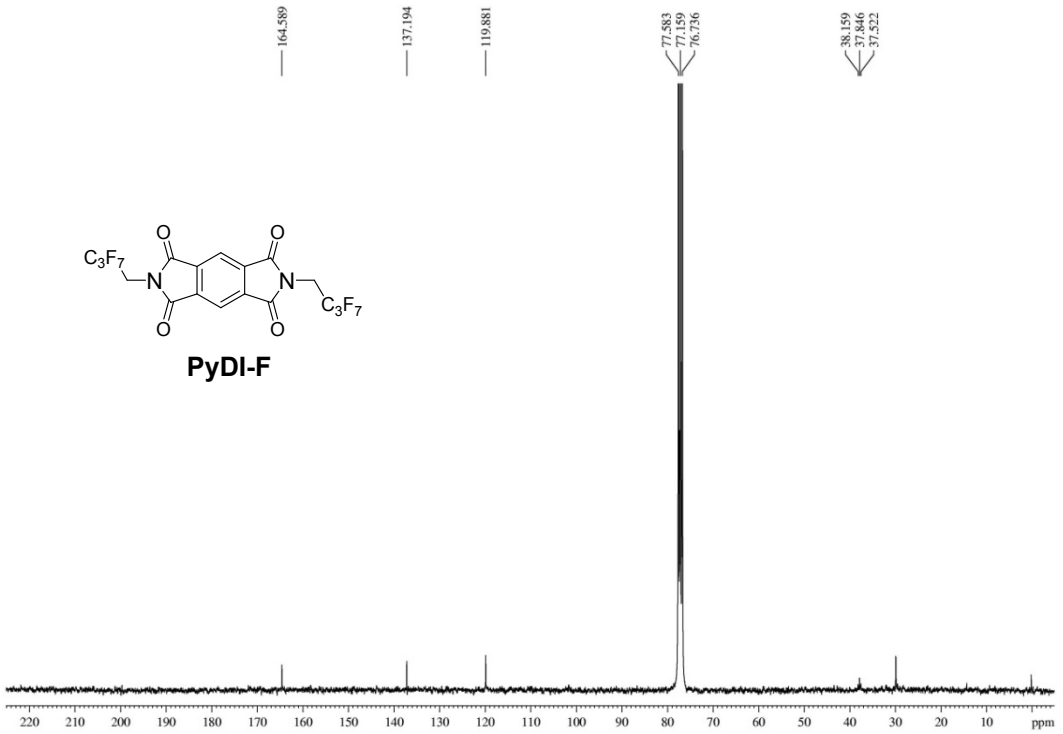



**Figure S4. $^{13}$C NMR spectra of PyDI-F.**

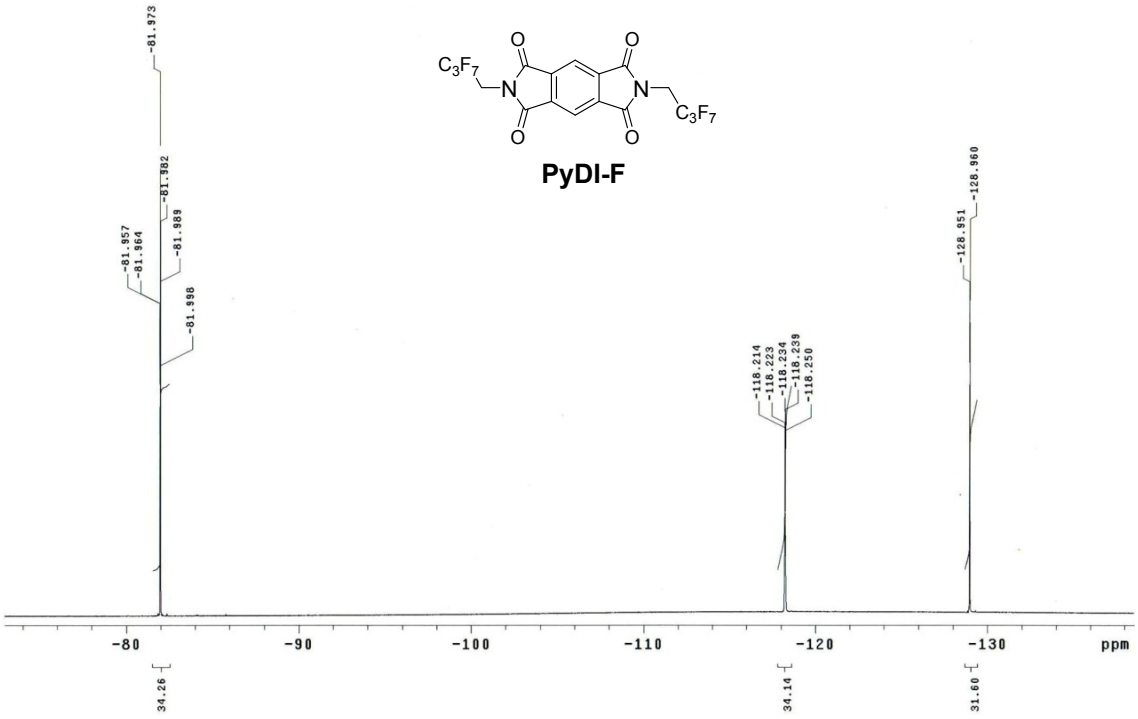



**Figure S5. $^{19}$F NMR spectra of PyDI-F.**

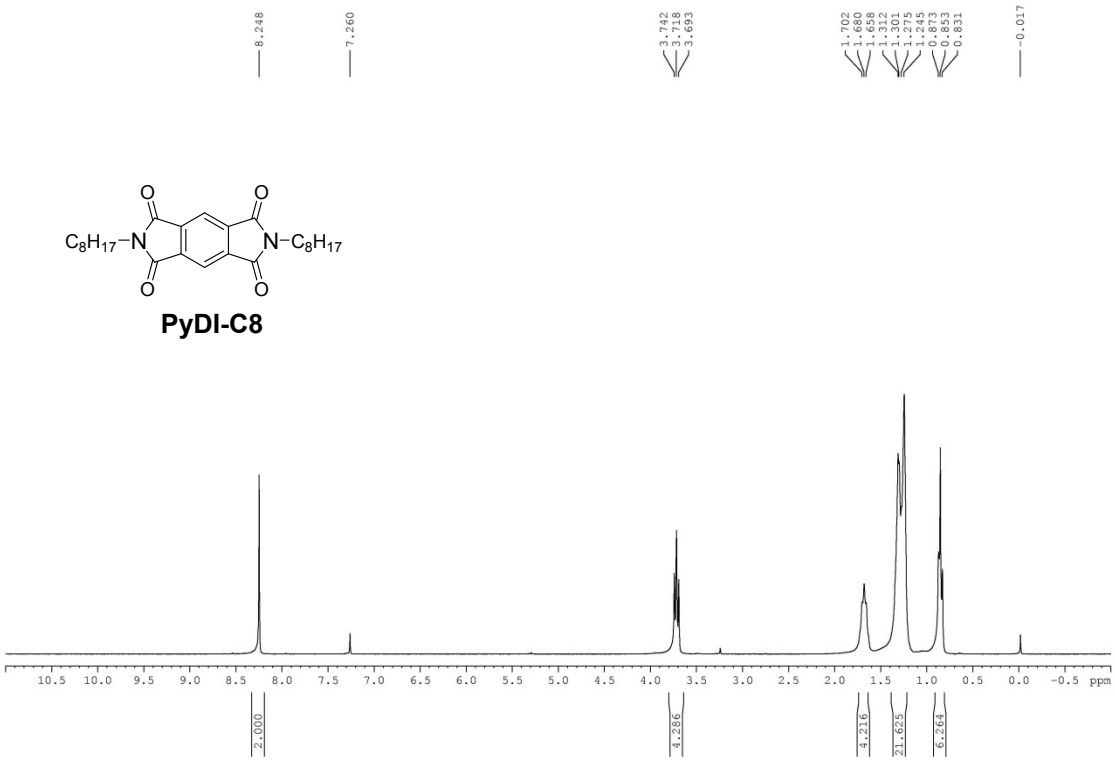



**Figure S6. $^{1}$H NMR spectra of PyDI-C8.**

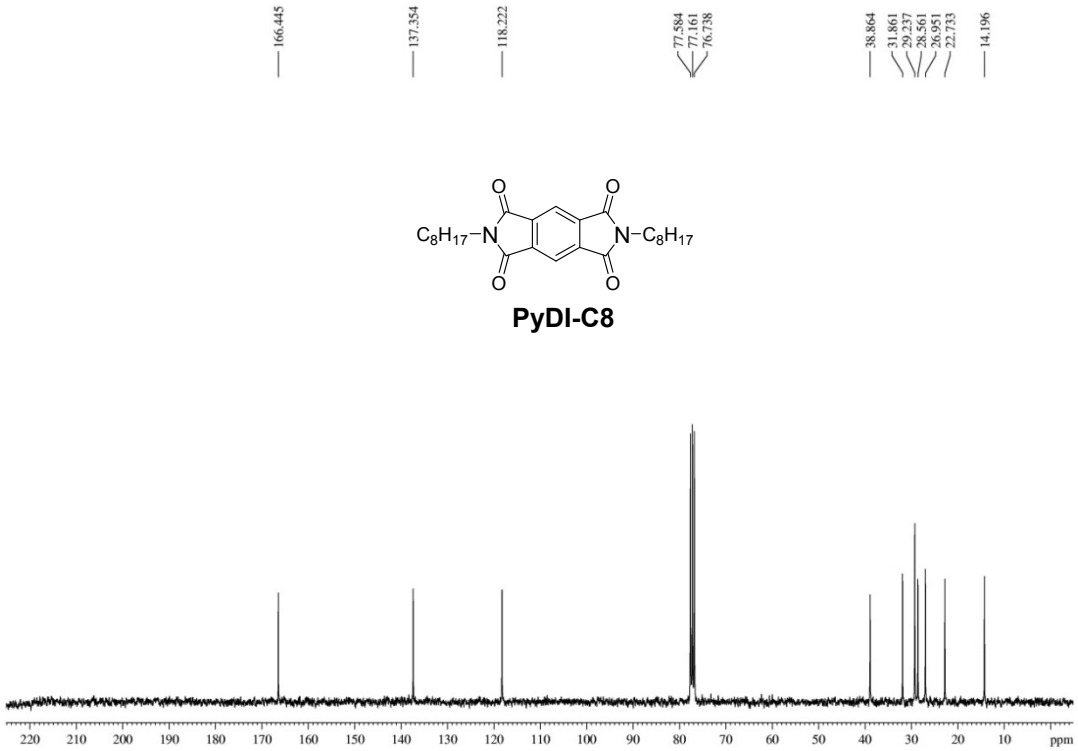



**Figure S7. $^{13}$C NMR spectra of PyDI-C8.**

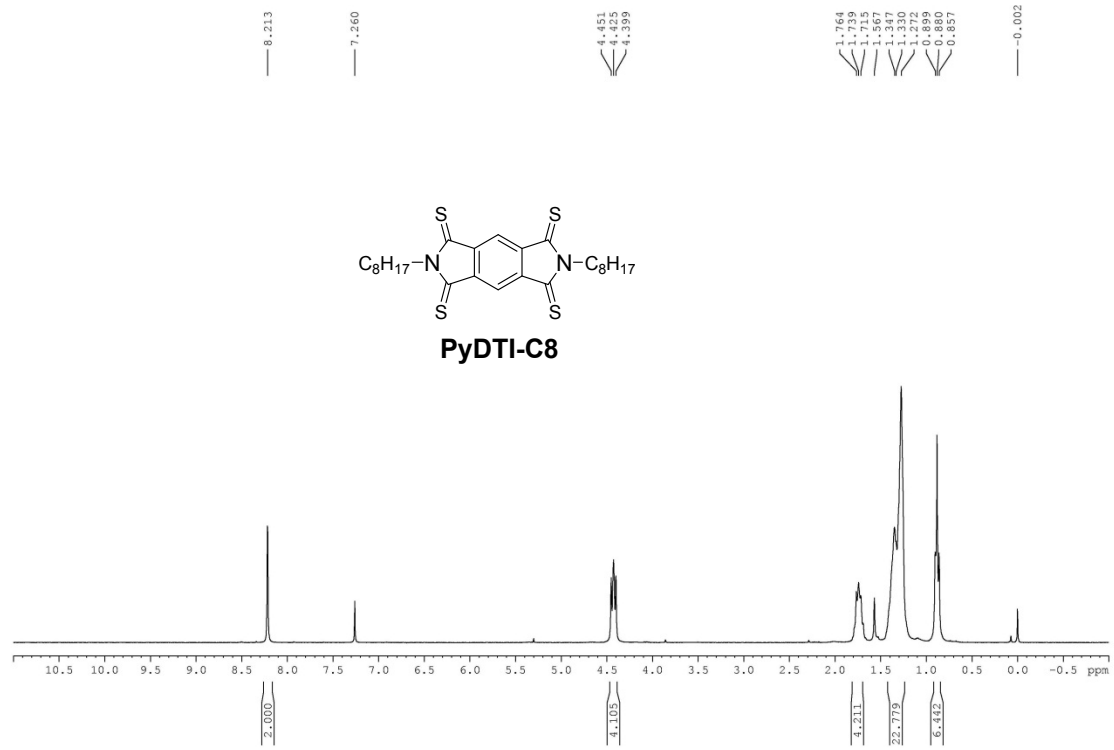



**Figure S8. $^{1}$H NMR spectra of PyDTI-C8.**

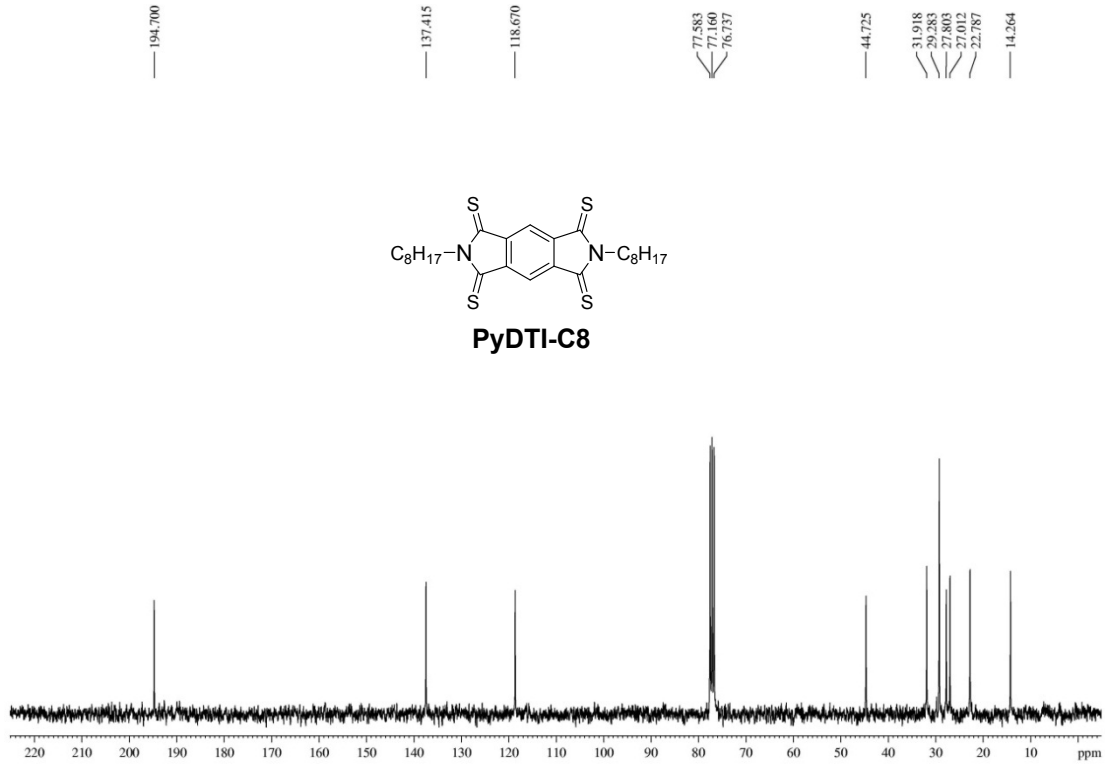



**Figure S9. $^{13}$C NMR spectra of PyDTI-C8.**

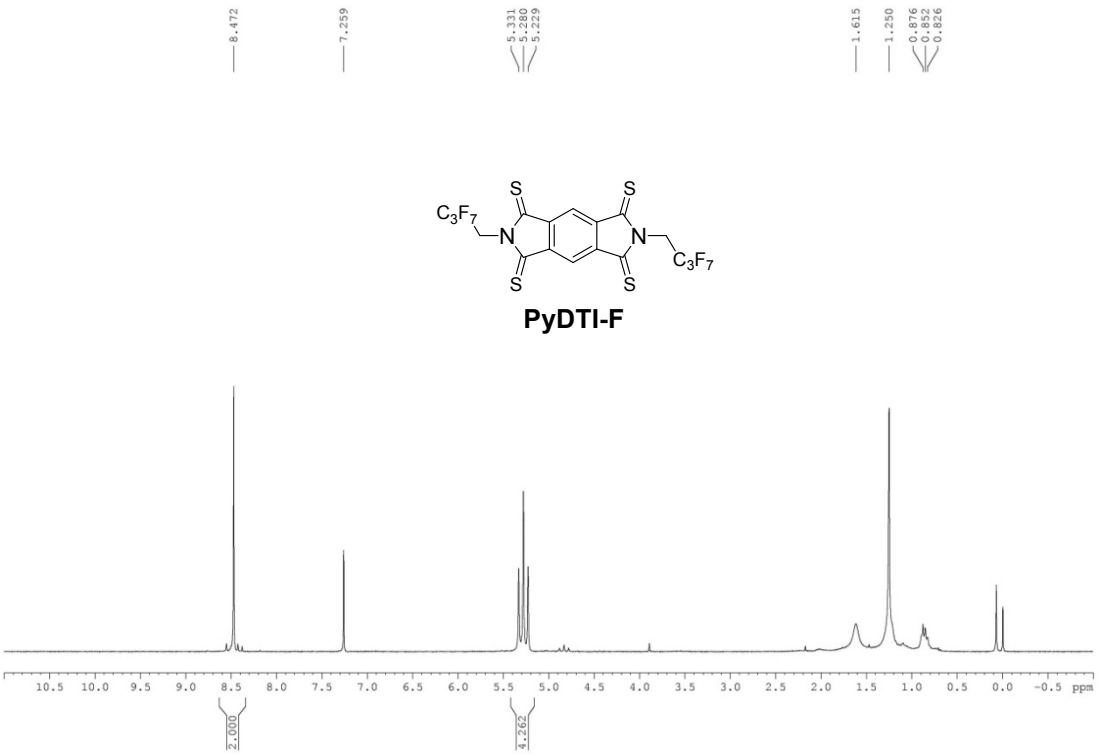



**Figure S10. $^{1}$H NMR spectra of PyDTI-F.**

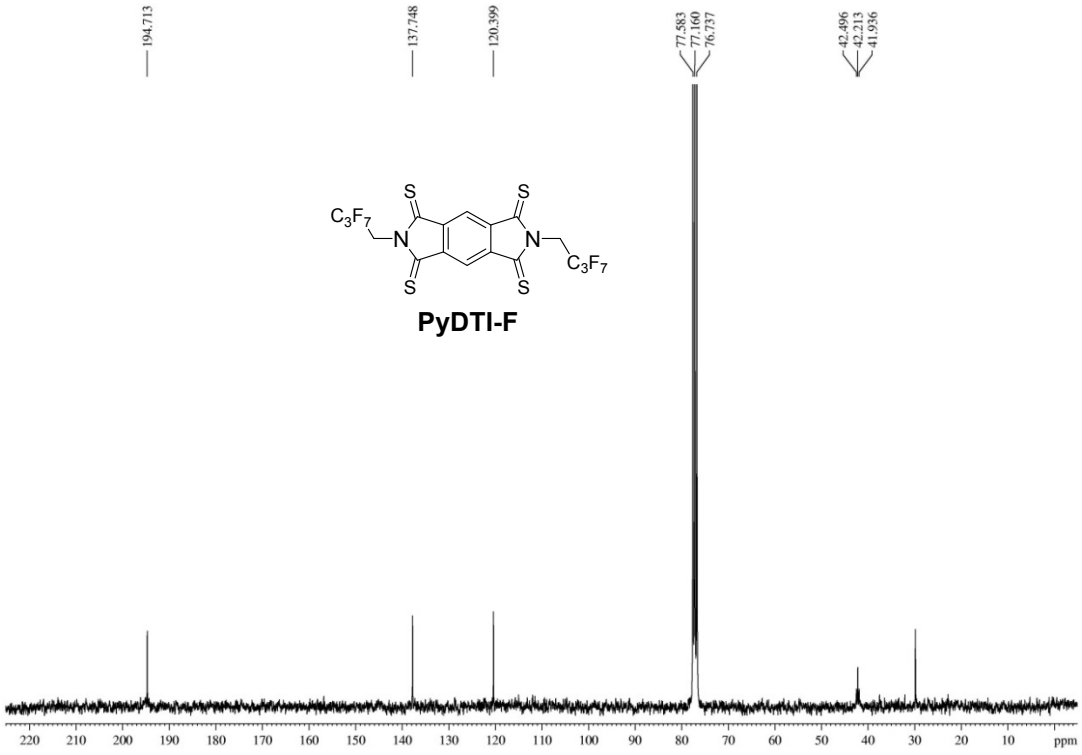



**Figure S11. $^{13}$C NMR spectra of PyDTI-F.**

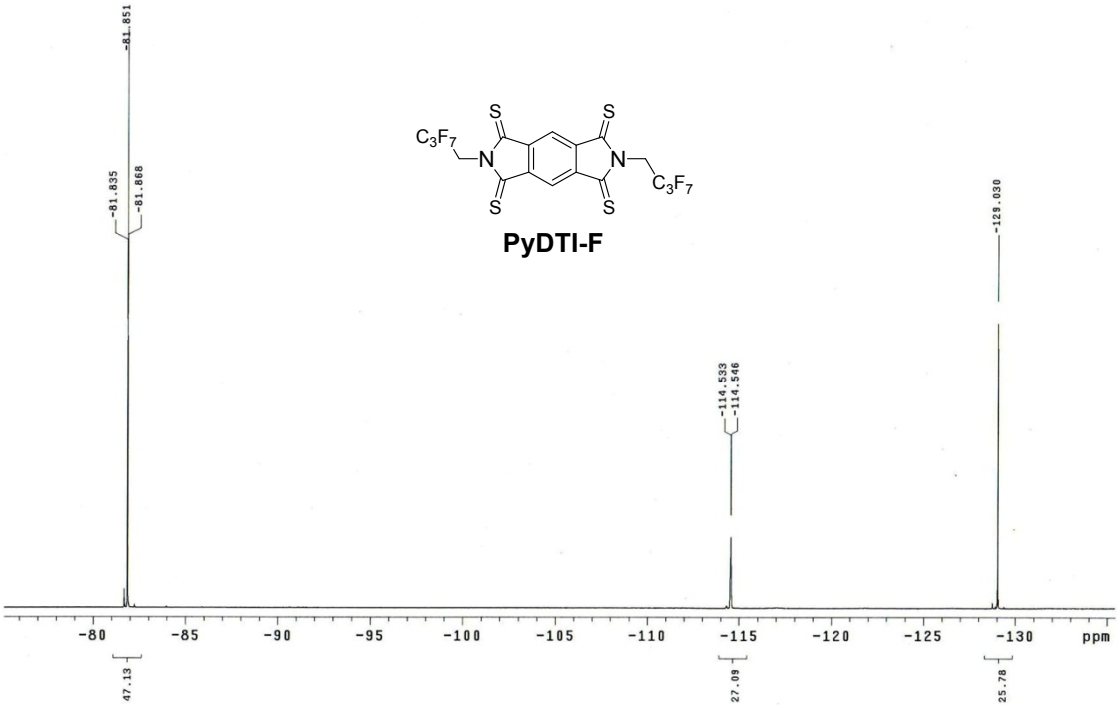



**Figure S12. $^{19}$F NMR spectra of PyDTI-F.**

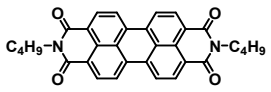
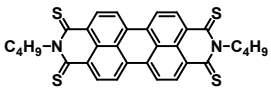
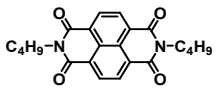
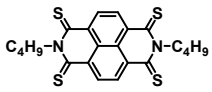
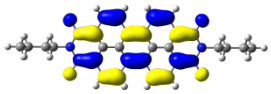
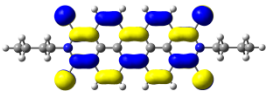
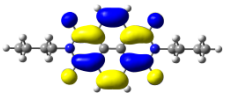
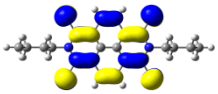
## 6. Computational

**The geometric optimizations and frequencies of PyDI-F and PyDTIs were calculated by density functional theory (DFT) at the B3LYP/6-31G** level with Gaussian 09 Program.[S4] The electronic couplings ($t$) of electron transfers were predicted by the Amsterdam density functional (ADF) program at PW91/TZ2P level, given by equation (1).[S5]**

$$t = \frac{H_{RP} - S_{RP}(H_{RR} + H_{PP})/2}{1 - S_{RP}^2} \quad \textbf{(1)}$$

**where $S_{RP}$ is spatial overlap, $H_{RP}$ is charge transfer integrals , and $H_{RR}$ and $H_{PP}$ are site energies.**

**Table S2. The LUMO levels and $\lambda^-$ values of PDI and NDI derivatives calculated at B3LYP/6-31G** level.**

| PDI-C4 | PDTI-C4 | NDI-C4 | NDTI-C4 |
|---|---|---|---|
|  |  |  |  |
| **LUMO: -3.44 eV** | **LUMO: -4.01 eV** | **LUMO: -3.37 eV** | **LUMO: -4.12 eV** |
|  |  |  |  |
| $\lambda^-$ = 271 meV | $\lambda^-$ = 205 meV | $\lambda^-$ = 378 meV | $\lambda^-$ = 227 meV |

**PyDI-F (B3LYP/6-31G**)**

**HF= -2497.7585157 (Hartree)**

**Cartesian Coordinates (Angstroms)**

| atom | X | Y | Z |
|---|---|---|---|
| C | -1.12854700 | -0.69559700 | -0.32087900 |
| C | 0.00002400 | -1.44418800 | 0.00005300 |
| C | 1.12856500 | -0.69551200 | 0.32088800 |
| C | 1.12852900 | 0.70558300 | 0.32143500 |
| C | -0.00003200 | 1.45416300 | -0.00014300 |
| C | -1.12856200 | 0.70549800 | -0.32162900 |
| C | 2.49083800 | -1.16674800 | 0.71780500 |
| C | 2.49098200 | 1.17655400 | 0.71969100 |
| O | 2.89049800 | 2.30794100 | 0.87970000 |
| O | 2.89061400 | -2.29826700 | 0.87650800 |
| C | -2.49082000 | -1.16693700 | -0.71766400 |
| O | -2.89054400 | -2.29849300 | -0.87624900 |
| C | -2.49102100 | 1.17636500 | -0.71999400 |
| O | -2.89060000 | 2.30771800 | -0.88007900 |
| N | 3.24835200 | 0.00465000 | 0.91373700 |

| | | | |
|---|---|---|---|
| **N** | **-3.24837000** | **0.00440700** | **-0.91379000** |
| **H** | **0.00003900** | **-2.52868000** | **0.00013700** |
| **H** | **-0.00004700** | **2.53866200** | **-0.00022700** |
| **C** | **4.63882900** | **0.00127000** | **1.30448600** |
| **C** | **-4.63885900** | **0.00087700** | **-1.30450100** |
| **C** | **5.55665900** | **0.00988200** | **0.07756900** |
| **C** | **7.05146600** | **-0.06242800** | **0.46390700** |
| **C** | **8.06813600** | **0.03272000** | **-0.69990800** |
| **C** | **-5.55665100** | **0.00989000** | **-0.07755700** |
| **C** | **-7.05146100** | **-0.06270000** | **-0.46381800** |
| **C** | **-8.06812300** | **0.03296700** | **0.69995700** |
| **H** | **4.83835700** | **-0.90094700** | **1.88557000** |
| **H** | **4.84216600** | **0.89048000** | **1.90298500** |
| **H** | **-4.83837500** | **-0.90154800** | **-1.88526200** |
| **H** | **-4.84224000** | **0.88987500** | **-1.90330200** |
| **F** | **5.35499900** | **1.14289200** | **-0.65014500** |
| **F** | **5.27135800** | **-1.05205300** | **-0.72403600** |
| **F** | **7.26258400** | **-1.23971900** | **1.10616700** |
| **F** | **7.31630500** | **0.95500900** | **1.32575700** |
| **F** | **7.99346100** | **1.23051200** | **-1.29067200** |
| **F** | **7.83138100** | **-0.92001700** | **-1.60973000** |
| **F** | **9.30523700** | **-0.13202900** | **-0.21247300** |
| **F** | **-5.35507400** | **1.14320500** | **0.64969500** |
| **F** | **-5.27122700** | **-1.05170400** | **0.72446400** |
| **F** | **-7.26252600** | **-1.24034400** | **-1.10547300** |
| **F** | **-7.31637200** | **0.95427600** | **-1.32617600** |
| **F** | **-7.99335900** | **1.23099800** | **1.29023400** |
| **F** | **-7.83144700** | **-0.91941000** | **1.61016900** |
| **F** | **-9.30523400** | **-0.13188000** | **0.21257800** |

**PyDTI-C8 (B3LYP/6-31G**)**

**HF= -2714.8451788 (Hartree)**

**Cartesian Coordinates (Angstroms)**

| atom | X | Y | Z |
|---|---|---|---|
| C | 1.11577554 | -0.59968242 | 0.37734114 |
| C | -0.00001070 | -1.34231938 | 0.00003765 |
| C | -1.11578501 | -0.59967577 | -0.37728713 |
| C | -1.11695353 | 0.80887780 | -0.37455596 |
| C | 0.00001411 | 1.55149395 | -0.00001043 |
| C | 1.11696743 | 0.80887134 | 0.37456424 |
| C | -2.44033404 | -1.05309057 | -0.83208860 |
| C | -2.44476807 | 1.26161169 | -0.82149939 |
| S | -2.97401230 | 2.81338030 | -0.99041418 |
| S | -2.96115361 | -2.60523326 | -1.02329131 |
| C | 2.44032097 | -1.05310524 | 0.83214547 |
| S | 2.96112234 | -2.60525197 | 1.02336574 |
| C | 2.44478986 | 1.26159678 | 0.82149460 |
| S | 2.97405434 | 2.81336091 | 0.99038756 |
| N | -3.17521193 | 0.10383362 | -1.07974621 |
| N | 3.17521588 | 0.10381567 | 1.07977228 |
| H | -0.00001968 | -2.42695611 | 0.00005551 |
| H | 0.00002281 | 2.63613701 | -0.00002756 |
| C | -4.56782776 | 0.10057369 | -1.53908655 |
| C | 4.56783990 | 0.10055004 | 1.53908935 |
| C | -5.57402145 | 0.04604364 | -0.38330902 |
| C | -7.02048047 | 0.03422555 | -0.89261605 |
| C | -8.05432687 | -0.07574727 | 0.23495557 |
| C | 5.57401780 | 0.04615686 | 0.38329164 |
| C | 7.02048185 | 0.03429171 | 0.89258101 |
| C | 8.05432364 | -0.07548813 | -0.23501629 |
| H | -4.68251213 | -0.77025514 | -2.18866002 |
| H | -4.70641128 | 1.00915704 | -2.12888944 |

| | | | |
|---|---|---|---|
| **H** | **4.68255441** | **-0.77034492** | **2.18856744** |
| **H** | **4.70641018** | **1.00907364** | **2.12898844** |
| **H** | **-5.41460972** | **0.91083792** | **0.27169736** |
| **H** | **-5.38277907** | **-0.85373189** | **0.21305282** |
| **H** | **-7.15392410** | **-0.80655413** | **-1.58783109** |
| **H** | **-7.21056290** | **0.94665616** | **-1.47470252** |
| **H** | **-7.91930417** | **0.76020166** | **0.93559677** |
| **H** | **-7.86145165** | **-0.99053811** | **0.81262049** |
| **C** | **-9.50322418** | **-0.08935371** | **-0.26723522** |
| **H** | **5.41458918** | **0.91101817** | **-0.27161957** |
| **H** | **5.38277537** | **-0.85355761** | **-0.21316221** |
| **H** | **7.15394961** | **-0.80658817** | **1.58766838** |
| **H** | **7.21055443** | **0.94664116** | **1.47480119** |
| **H** | **7.91924316** | **0.76054606** | **-0.93554493** |
| **H** | **7.86149722** | **-0.99021574** | **-0.81279668** |
| **C** | **9.50322343** | **-0.08906337** | **0.26716757** |
| **C** | **-10.53900233** | **-0.23037024** | **0.85457518** |
| **C** | **-11.98817211** | **-0.24619352** | **0.35291597** |
| **C** | **-13.01621566** | **-0.39881465** | **1.47775302** |
| **C** | **10.53898868** | **-0.23048084** | **-0.85460540** |
| **C** | **11.98816021** | **-0.24618308** | **-0.35294849** |
| **C** | **13.01619819** | **-0.39915412** | **-1.47774306** |
| **H** | **-9.63028657** | **-0.91422974** | **-0.98288229** |
| **H** | **-9.70093078** | **0.83329378** | **-0.83117873** |
| **H** | **9.63022973** | **-0.91373543** | **0.98305970** |
| **H** | **9.70100354** | **0.83373739** | **0.83083358** |
| **H** | **-10.41341931** | **0.59289397** | **1.57251328** |
| **H** | **-10.34102395** | **-1.15400932** | **1.41710230** |
| **H** | **-12.11133807** | **-1.06525866** | **-0.36873963** |
| **H** | **-12.18815767** | **0.67948944** | **-0.20369470** |
| **H** | **-12.94242506** | **0.42455821** | **2.19734436** |

| | | | |
|---|---|---|---|
| **H** | **-12.86300413** | **-1.33297396** | **2.02996231** |
| **H** | **-14.03906855** | **-0.40776746** | **1.08750132** |
| **H** | **10.41342693** | **0.59255328** | **-1.57281107** |
| **H** | **10.34097611** | **-1.15429660** | **-1.41682956** |
| **H** | **12.11131478** | **-1.06503595** | **0.36895008** |
| **H** | **12.18816444** | **0.67966129** | **0.20338691** |
| **H** | **12.94242157** | **0.42401118** | **-2.19757295** |
| **H** | **12.86296730** | **-1.33347070** | **-2.02968114** |
| **H** | **14.03905146** | **-0.40801287** | **-1.08749039** |

**PyDTI-F (B3LYP/6-31G**)**

**HF= -3789.5847747 (Hartree)**

**Cartesian Coordinates (Angstroms)**

| **atom** | **X** | **Y** | **Z** |
|---|---|---|---|
| **C** | **1.13773802** | **0.71927078** | **-0.30632291** |
| **C** | **0.00002397** | **1.46159308** | **-0.00008165** |
| **C** | **-1.13770520** | **0.71928645** | **0.30614422** |
| **C** | **-1.13762441** | **-0.69007812** | **0.30576980** |
| **C** | **0.00000106** | **-1.43239224** | **-0.00009311** |
| **C** | **1.13763791** | **-0.69009327** | **-0.30595420** |
| **C** | **-2.48286779** | **1.17962480** | **0.68145226** |
| **C** | **-2.48237261** | **-1.15098565** | **0.68044707** |
| **S** | **-2.99171347** | **-2.69629841** | **0.91014555** |
| **S** | **-2.99254497** | **2.72452764** | **0.91272954** |
| **C** | **2.48291737** | **1.17958909** | **-0.68160315** |
| **S** | **2.99262245** | **2.72447970** | **-0.91290843** |
| **C** | **2.48239230** | **-1.15102153** | **-0.68057405** |
| **S** | **2.99172302** | **-2.69634175** | **-0.91023785** |
| **N** | **-3.24044747** | **0.01399516** | **0.85069732** |
| **N** | **3.24048624** | **0.01395480** | **-0.85081368** |
| **H** | **0.00003192** | **2.54620597** | **-0.00007320** |

| | | | |
|---|---|---|---|
| **H** | **-0.00000473** | **-2.51699183** | **-0.00009426** |
| **C** | **-4.64339938** | **0.01142813** | **1.22071276** |
| **C** | **4.64345855** | **0.01136617** | **-1.22075068** |
| **C** | **-5.56076921** | **0.01204775** | **-0.00867485** |
| **C** | **-7.05250998** | **-0.07387586** | **0.39341291** |
| **C** | **-8.08040202** | **0.01703682** | **-0.76141123** |
| **C** | **5.56075397** | **0.01209910** | **0.00869625** |
| **C** | **7.05251273** | **-0.07394193** | **-0.39327592** |
| **C** | **8.08033588** | **0.01706512** | **0.76159813** |
| **H** | **-4.85055885** | **0.90425888** | **1.81154688** |
| **H** | **-4.84518256** | **-0.88885148** | **1.80313665** |
| **H** | **4.85064617** | **0.90415947** | **-1.81163273** |
| **H** | **4.84527937** | **-0.88895158** | **-1.80309955** |
| **F** | **-5.27710188** | **-1.04541862** | **-0.81571362** |
| **F** | **-5.38056129** | **1.14418277** | **-0.74246697** |
| **F** | **-7.31785369** | **0.93852091** | **1.26068772** |
| **F** | **-7.24833933** | **-1.25465273** | **1.03320644** |
| **F** | **-7.84330061** | **-0.92944036** | **-1.67750244** |
| **F** | **-8.02276494** | **1.21803983** | **-1.34726033** |
| **F** | **-9.31106420** | **-0.16159868** | **-0.26277972** |
| **F** | **5.27697592** | **-1.04525277** | **0.81585822** |
| **F** | **5.38055690** | **1.14433479** | **0.74232707** |
| **F** | **7.31794646** | **0.93831267** | **-1.26067414** |
| **F** | **7.24834499** | **-1.25483184** | **-1.03288791** |
| **F** | **7.84322330** | **-0.92936309** | **1.67773024** |
| **F** | **8.02261745** | **1.21810480** | **1.34737365** |
| **F** | **9.31103181** | **-0.16154507** | **0.26303733** |

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