Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting Information

Solution Processable Low Band Gap Diketopyrrolopyrrole (DPP) Based Derivatives: Novel Acceptors for Organic Solar Cells

Prashant Sonar[1*], Ging-MengNg[1], Ting Ting Lin[1], Ananth Dodabalapur[1,2] and Zhi-Kuan Chen[1*]
1. Institute of Materials Research and Engineering, 3 Research Link Singapore 117602, Republic of Singapore.
2. *Permanent Address:* Microelectronics Research Center, University of Texas at Austin, Austin, TX, 78758, USA.

Email: sonarp@imre.a-star.edu.sg, zk-chen@imre.a-star.edu.sg

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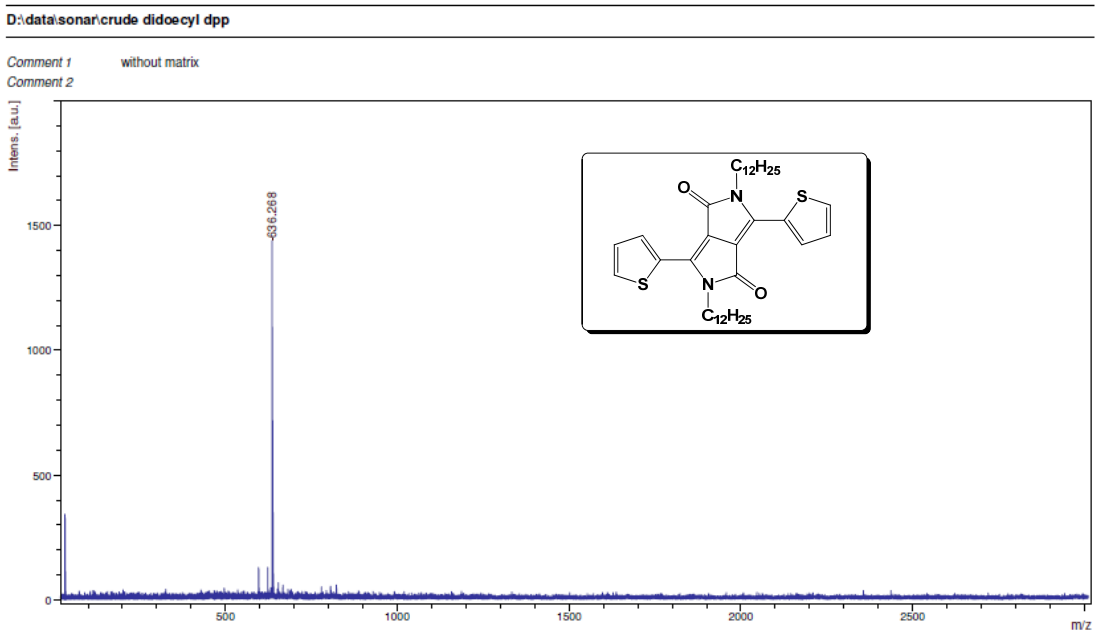
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S
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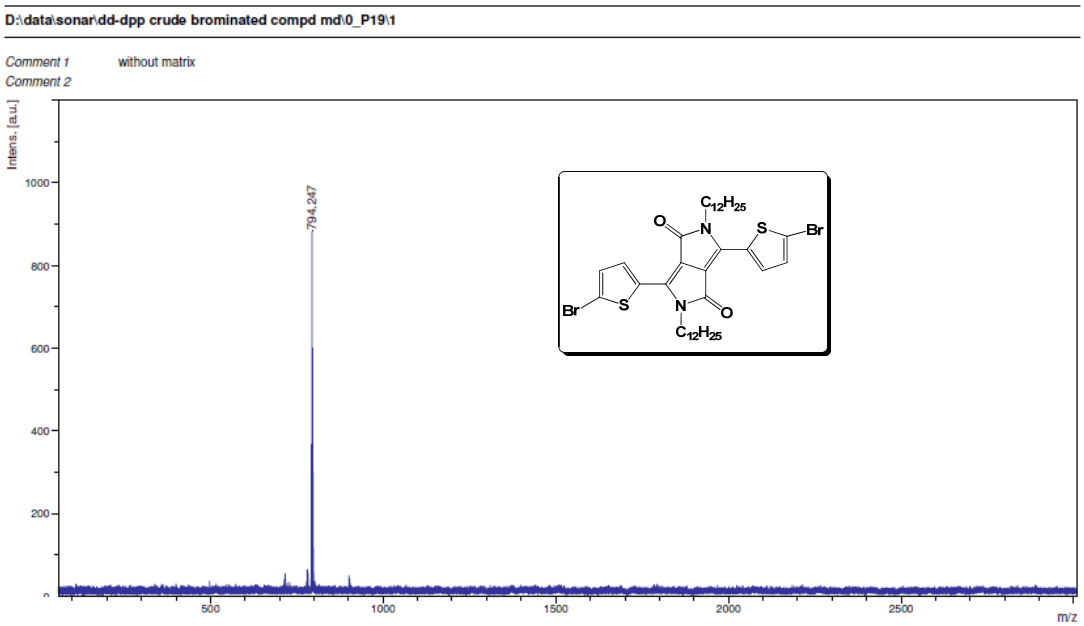
N
O
C12H25

(b)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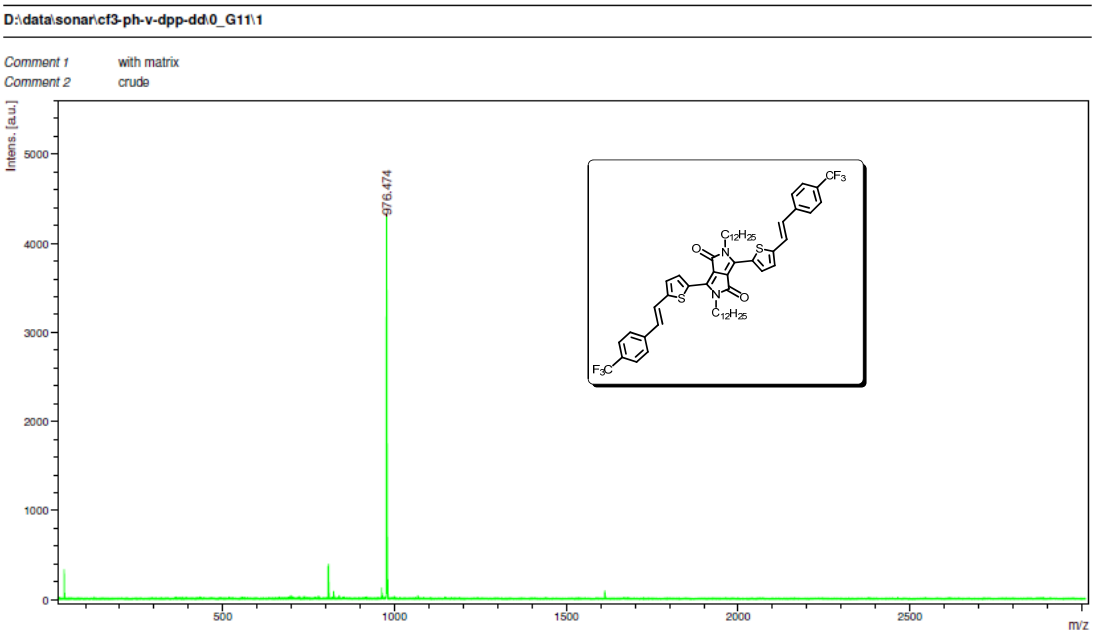
O
C12H25

(c)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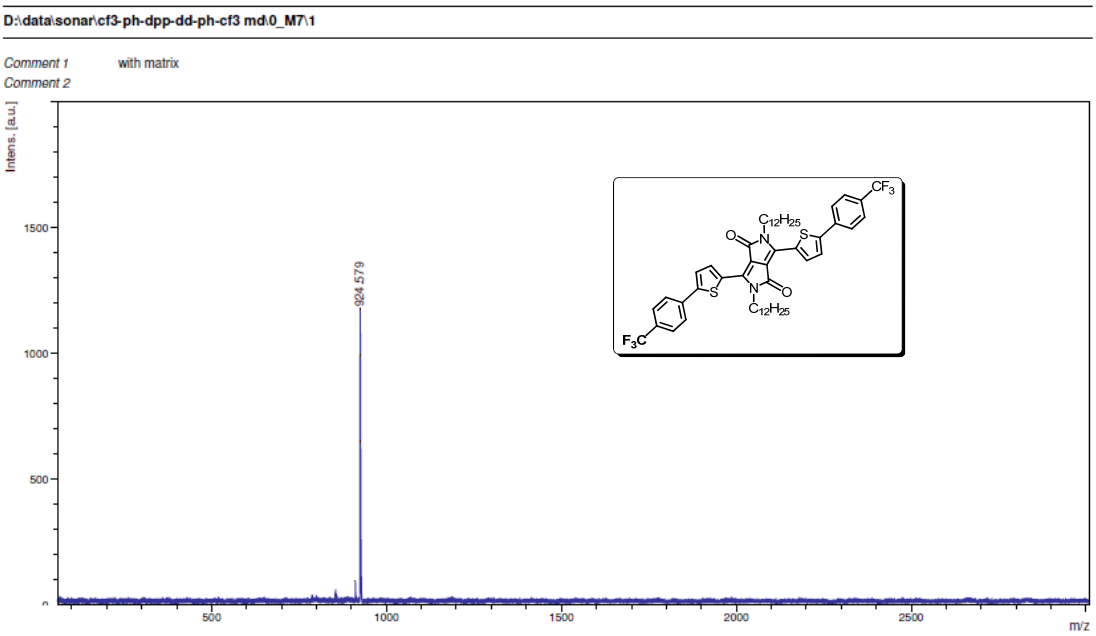
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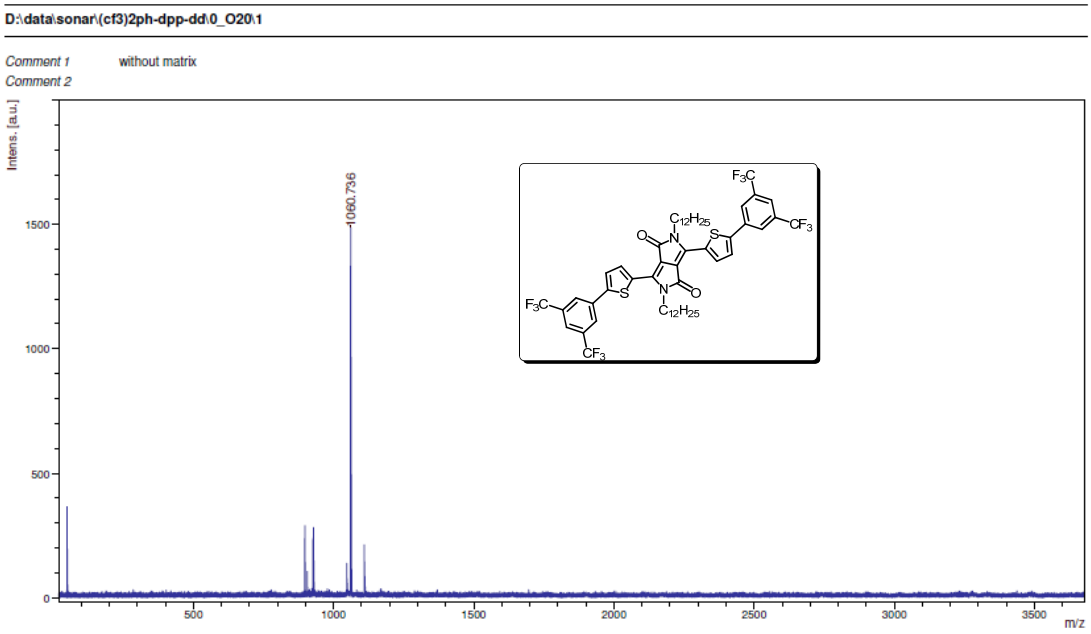
m/z

(e)



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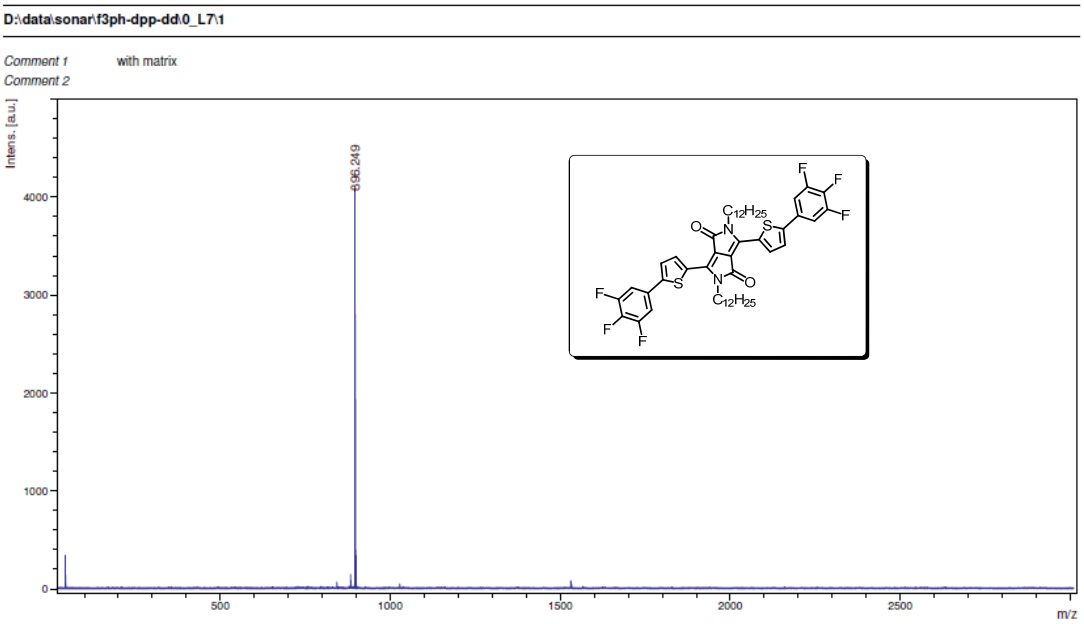
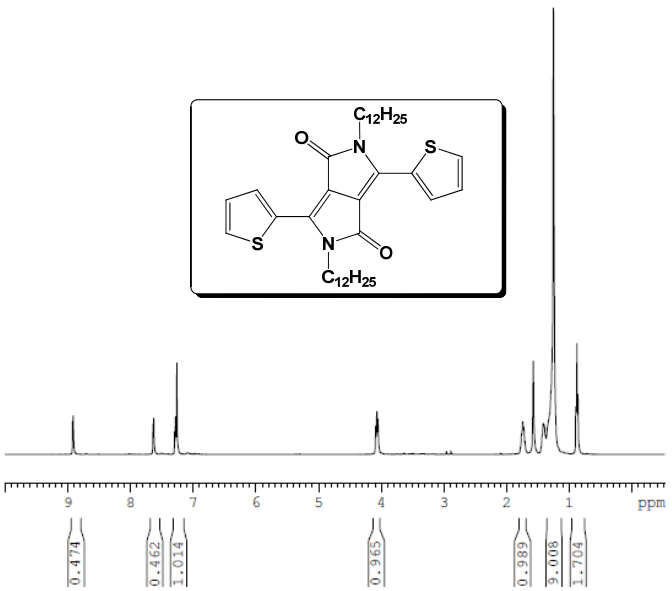


Fig.1 MALDI-TOF Spectrum of (a) N,N'-bis(dodecyl)-3,6-dithienyl-1,4-diketopyrrolo[3,4-c]pyrrole, (b) 3, 6-Bis- (5-bromo-thiophen-2-yl)-N, N'-bis (dodecyl)-1, 4-dioxo-pyrrolo [3, 4-c] pyrrole, (c) **TFPVDPP**, (d) **TFPDPP,** (e) **DTFPDPP** and (f) **F3PDPP**.

(a)



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PROCNO 1

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PULPROG z
TD 3276
SOLVENT CDCl
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FIDRES 0.158894
AQ 3.145777
RG 203.
DW 96.00
DE 6.0
TE 0.
D1 5.0000000
MCREST 0.0000000
MCWRK 0.0150000

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PL1 -2.0
SFO1 400.132400

F2 - Processing parame
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WDW E
SSB
LB 1.0
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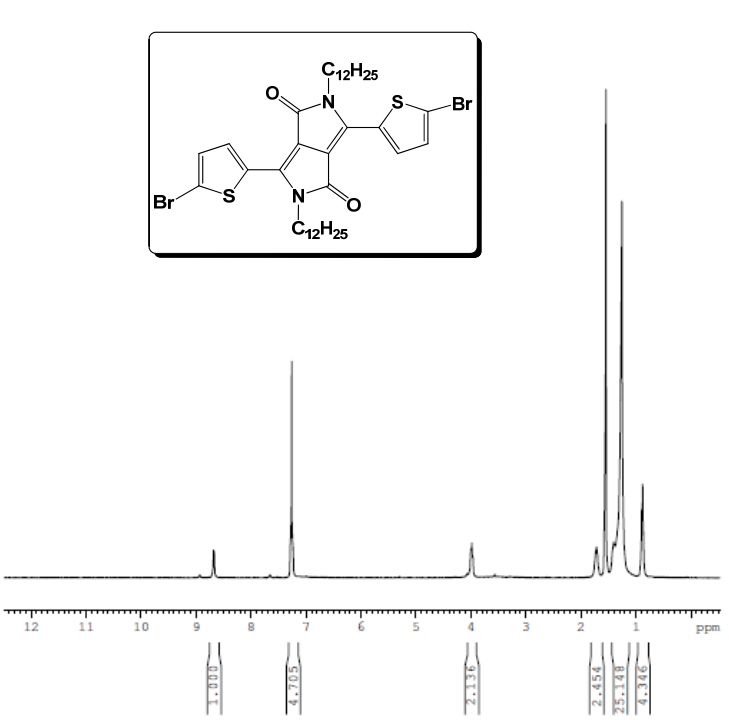
(b)



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PROCNO 1

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SOLVENT CDCl3
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FIDRES 0.158946 Hz
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DE 6.00 usec
TE 0.0 K
D1 5.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======= CHANNEL f1 =======
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P1 7.20 usec
PL1 -2.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
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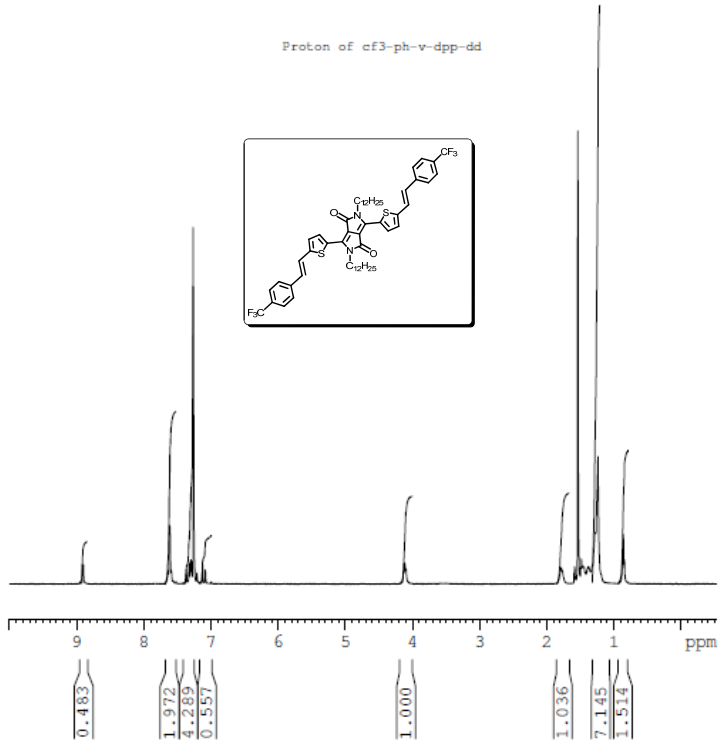
(c)

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PULPROG               zg
TD                 32768
SOLVENT            CDC13
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DE              6.00 usec
TE                 0.0 K
D1          5.00000000 sec
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MCWRK       0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 7.20 usec
PL1               -2.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
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SF          400.1300092 MHz
WDW                   EM
SSB                    0
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GB                     0
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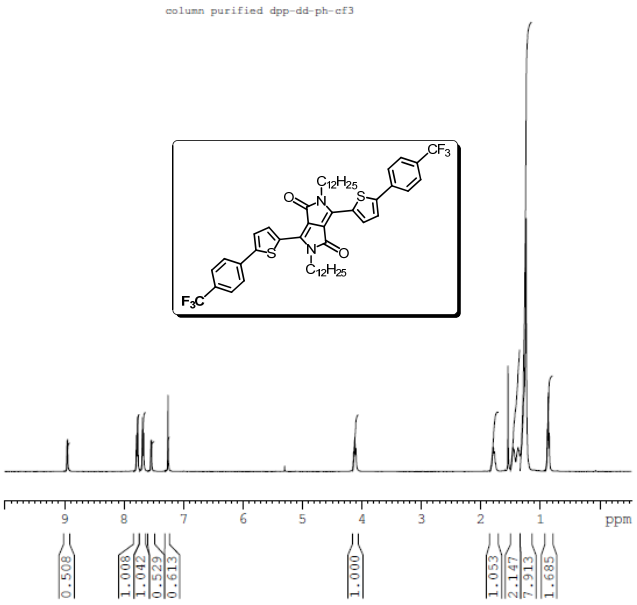
(d)

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TD                 32768
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MCWRK       0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 7.20 usec
PL1               -2.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
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SF          400.1300092 MHz
WDW                   EM
SSB                    0
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GB                     0
PC                1.00
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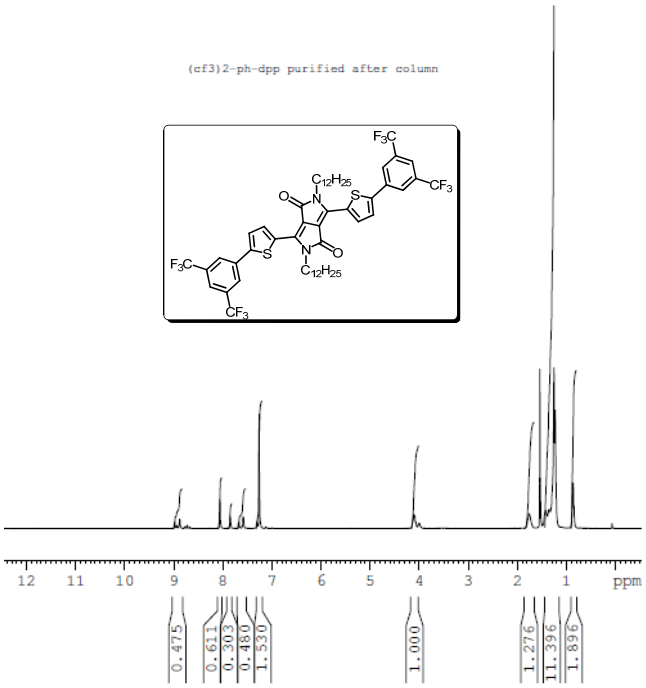
(e)

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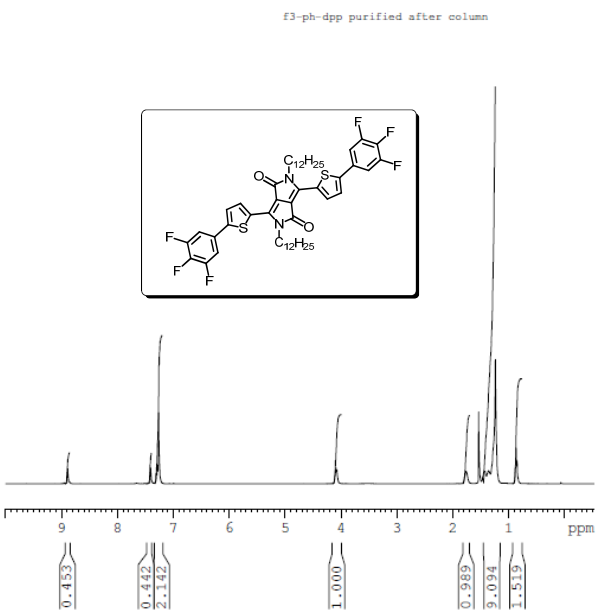
PULPROG                 zg
TD                   32768
SOLVENT              CDC13
NS                      16
DS                       0
SWH              5208.333 Hz
FIDRES           0.158946 Hz
AQ               3.1457779 sec
RG                     362
DW                96.000 usec
DE                 6.00 usec
TE                  0.0 K
D1              5.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   7.20 usec
PL1                 -2.00 dB
SFO1          400.1324008 MHz

F2 - Processing parameters
SI                   16384
SF            400.1300092 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.00
```

(f)

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DE                 6.00 usec
TE                  0.0 K
D1              5.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   7.20 usec
PL1                 -2.00 dB
SFO1          400.1324008 MHz

F2 - Processing parameters
SI                   16384
SF            400.1300092 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.00
```
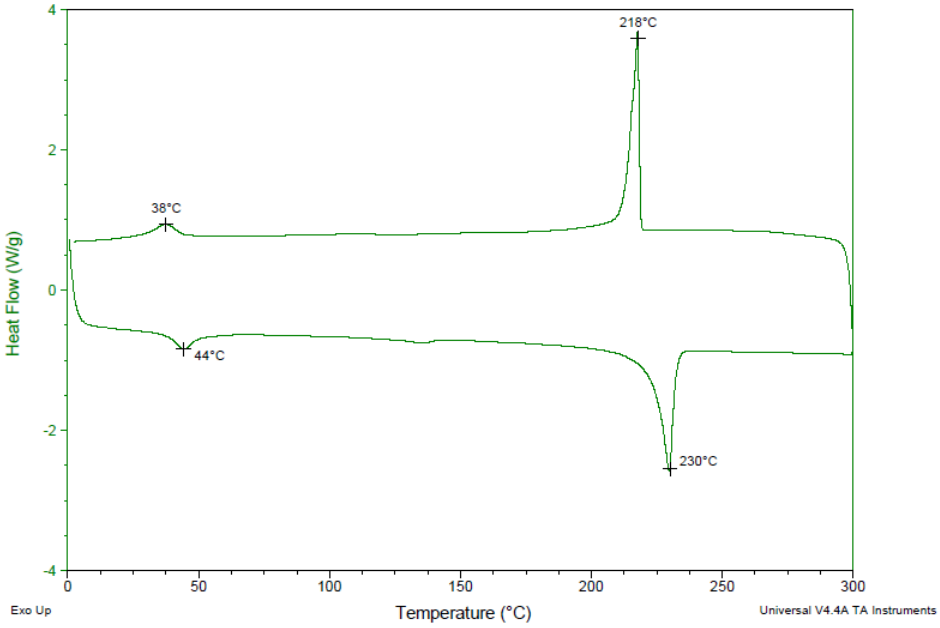

Fig. 2 NMR Spectrum of (a) N,N'-bis(dodecyl)-3,6-dithienyl-1,4-diketopyrrolo[3,4-c]pyrrole, (b) 3, 6-Bis- (5-bromo-thiophen-2-yl)-N, N'-bis (dodecyl)-1, 4-dioxo-pyrrolo [3, 4-c] pyrrole, (c) **TFPVDPP**, (d) **TFPDPP,** (e) **DTFPDPP** and (f) **F3PDPP** .

(a)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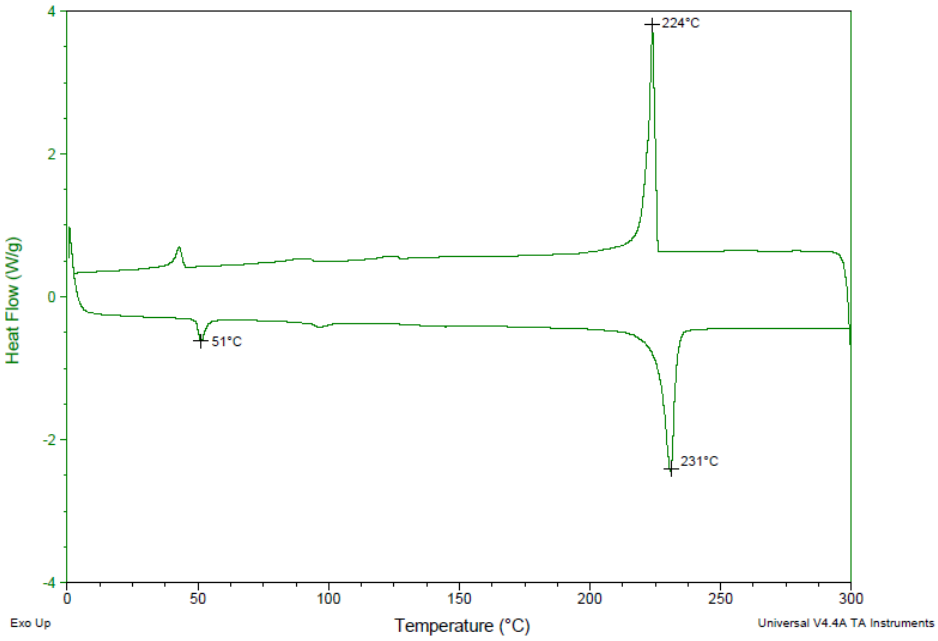
44°C
230°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.4A TA Instruments

(b)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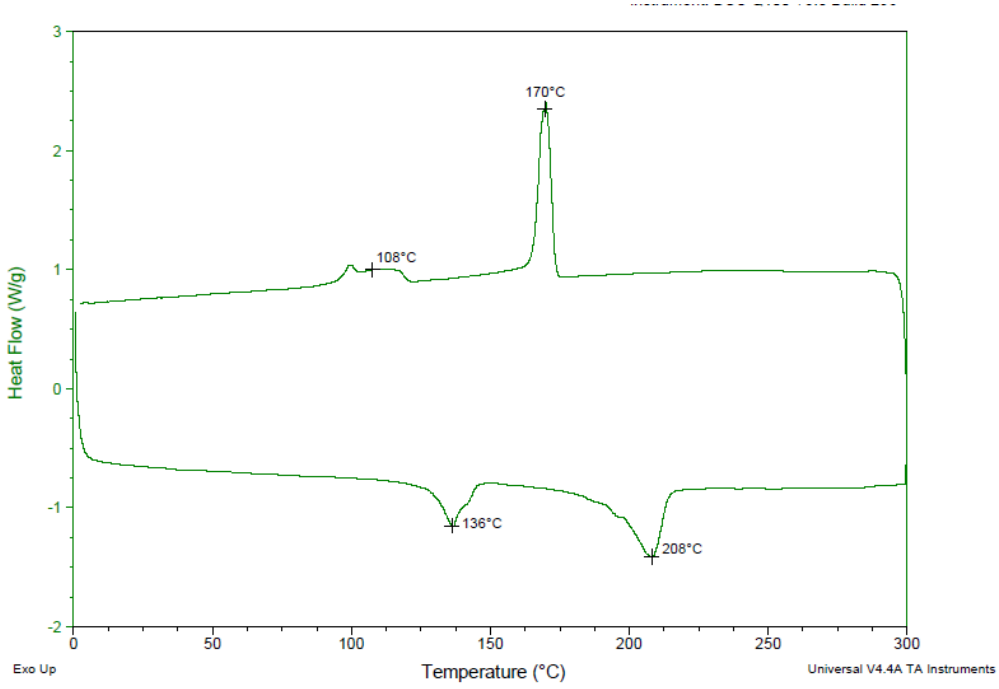
51°C
231°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.4A TA Instruments

(c)



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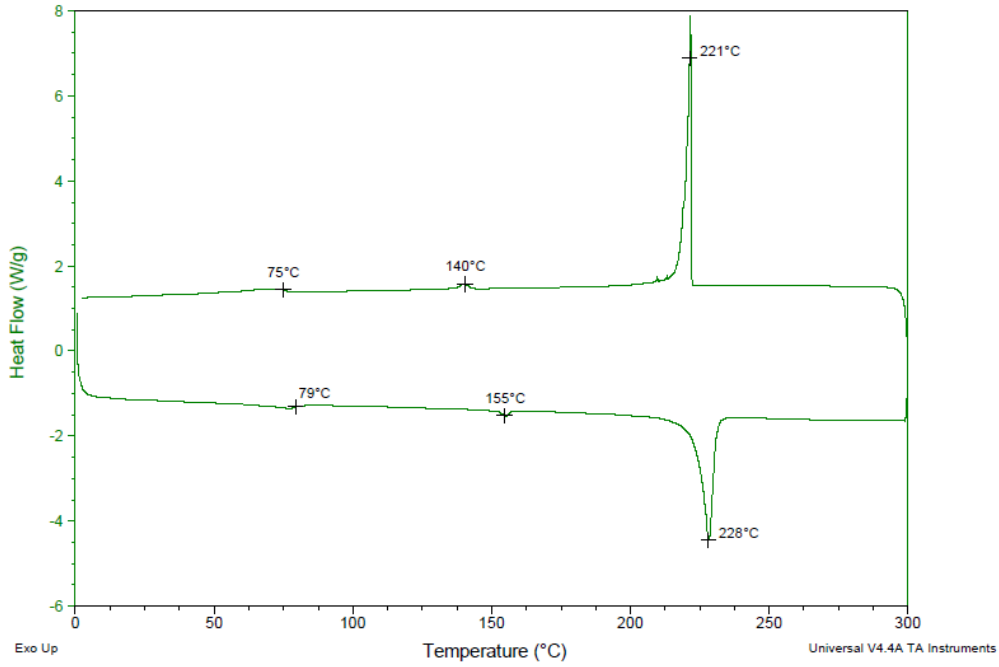
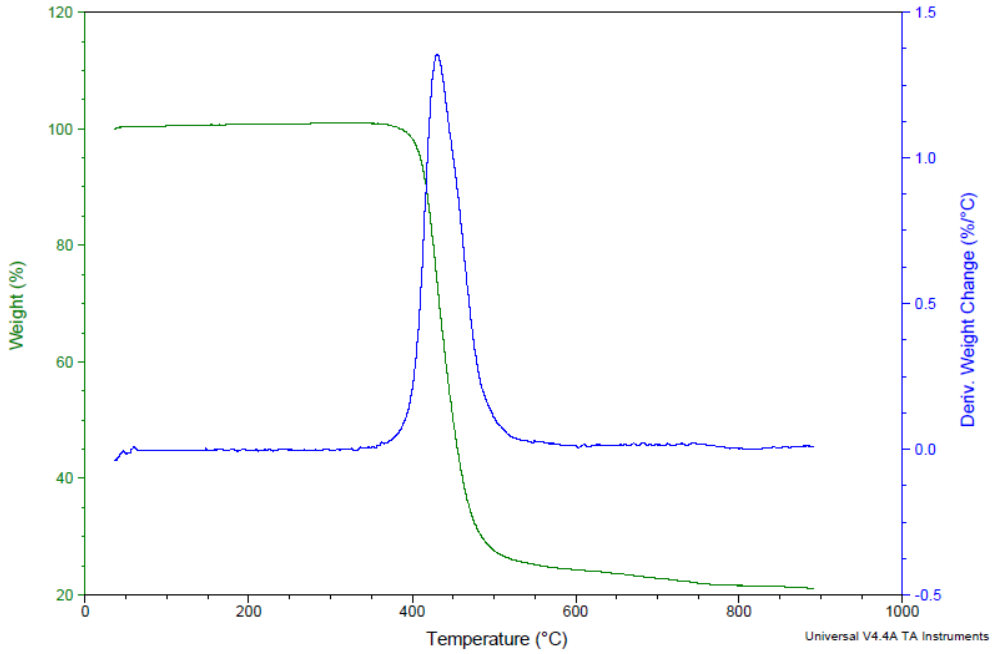


Fig.3 DSC Spectrum of (a) **TFPVDPP**, (b) **TFPDPP, (c) DTFPDPP** and **(f) F3PDPP** .

(a)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Deriv. Weight Change (%/°C)
Temperature (°C)
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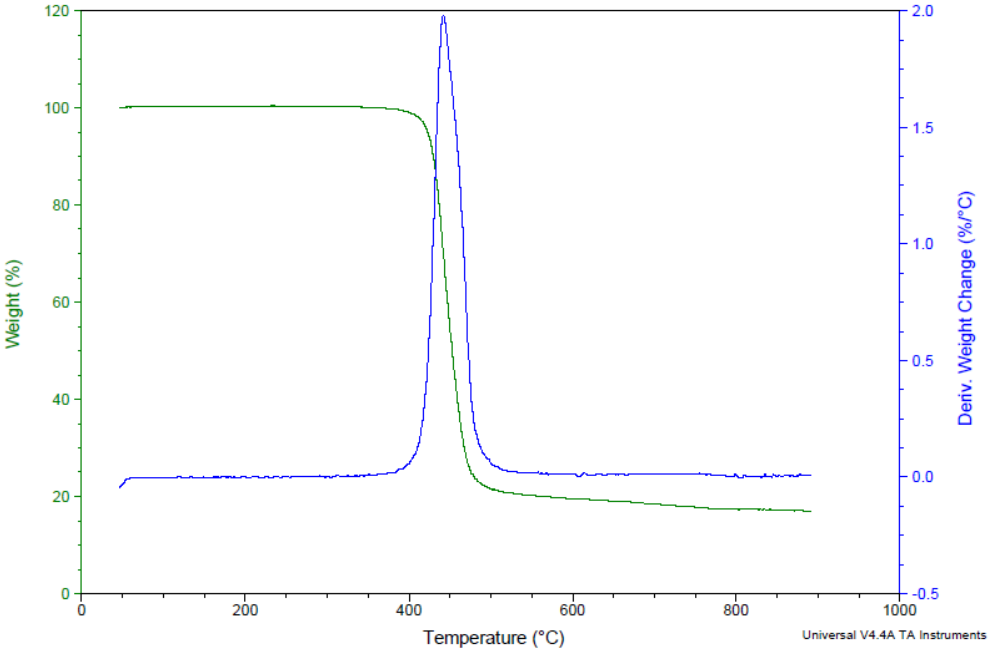
(b)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Universal V4.4A TA Instruments

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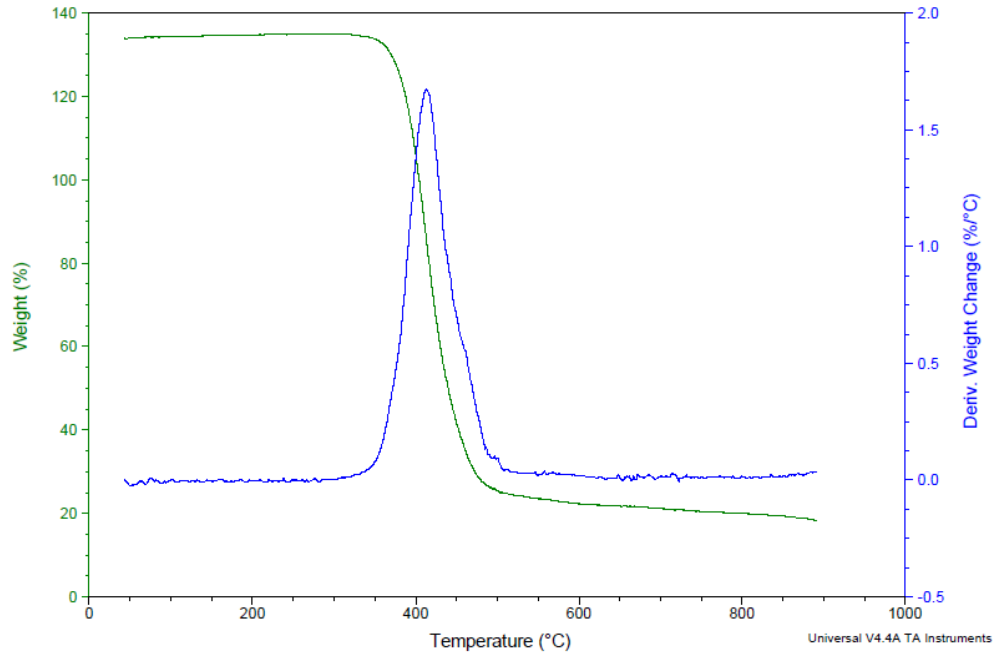

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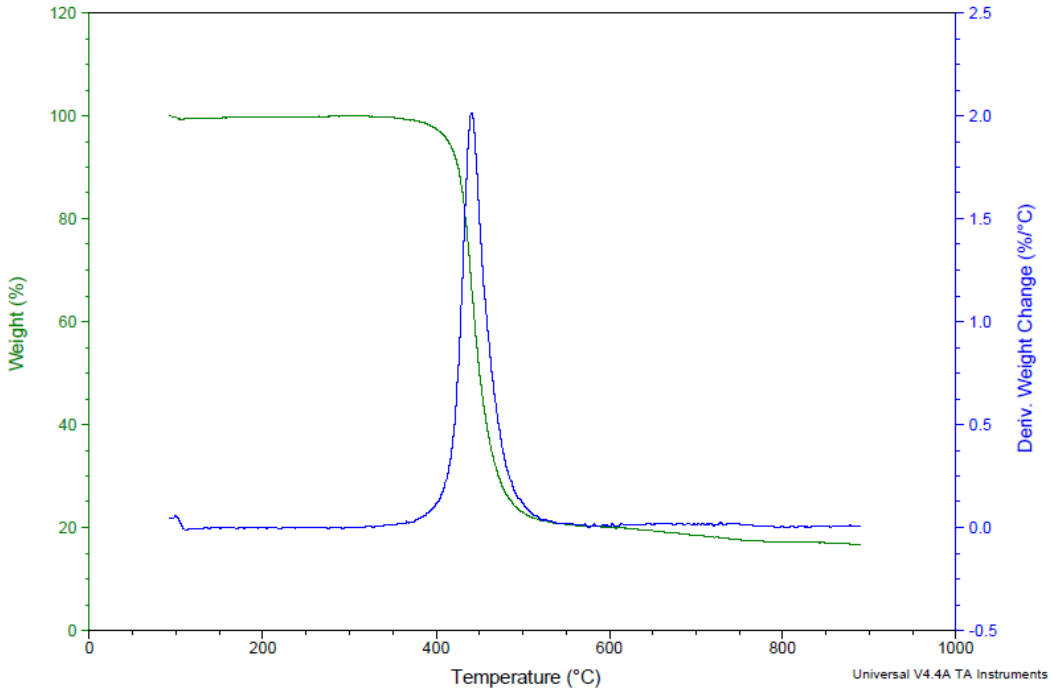
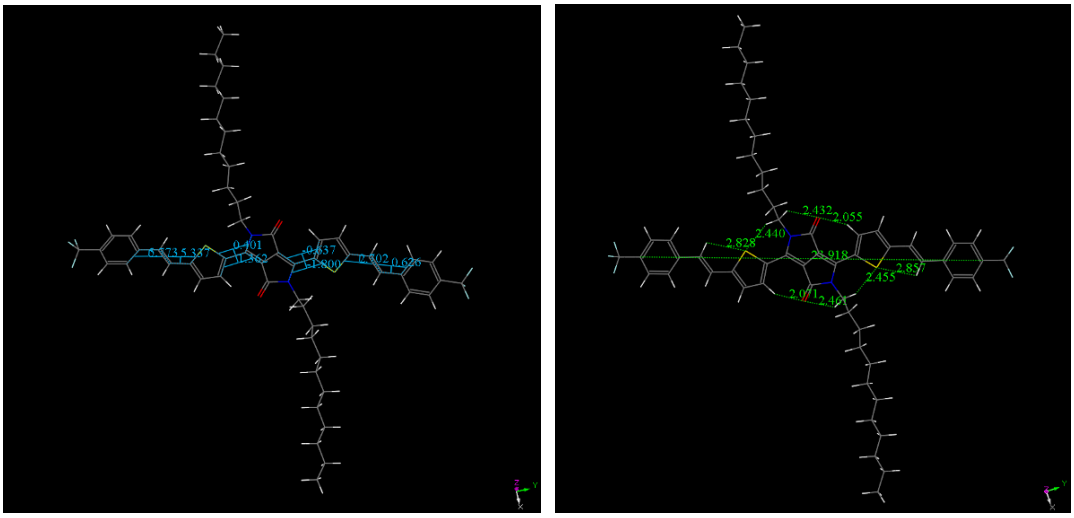


Fig.4 TGA Spectrum of (a) **TFPVDPP**, (b) **TFPDPP,** (c) **DTFPDPP** and (d) **F3PDPP** .

(a)



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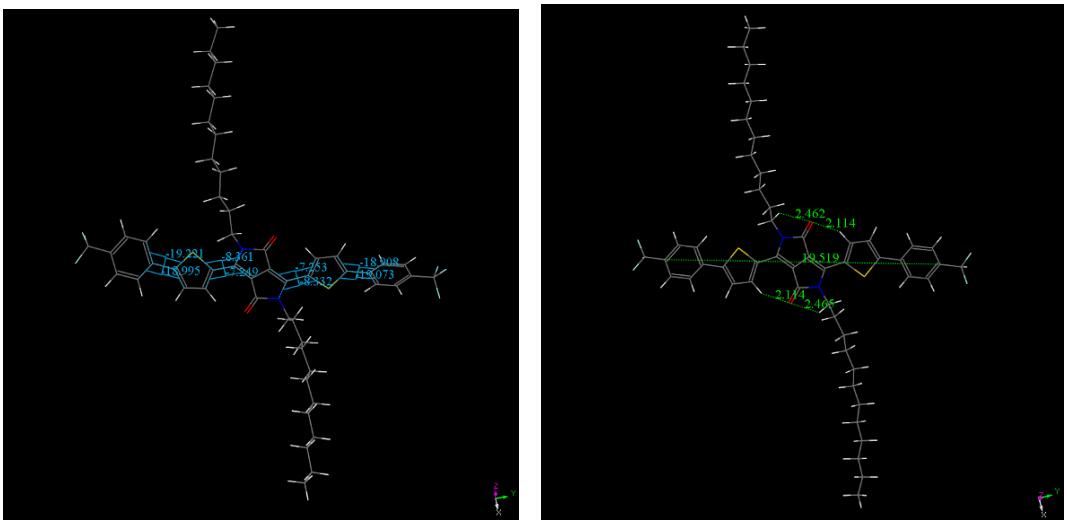

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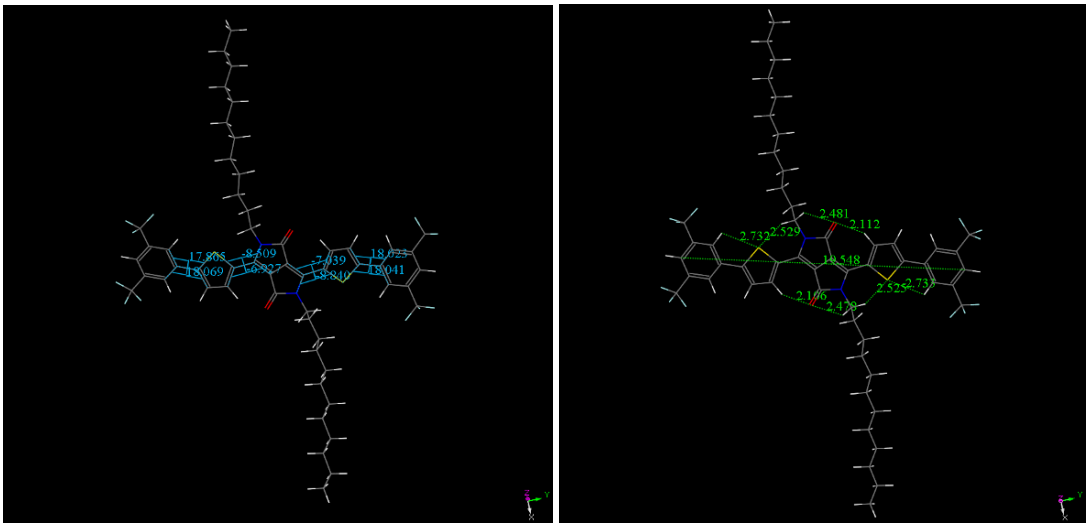

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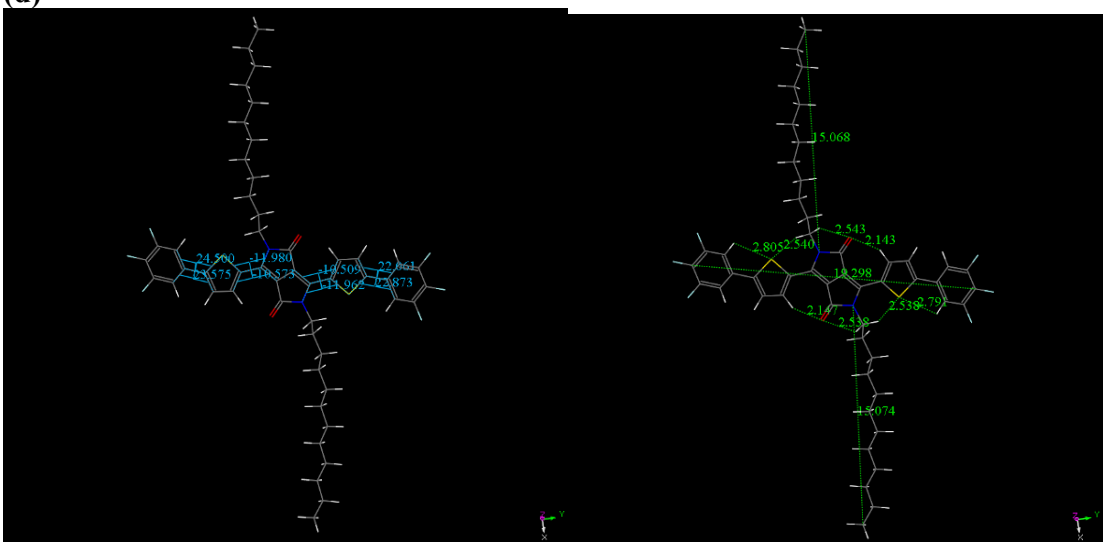

Fig.5 Dihedral angles and H—O distance for the optimized structures of **TFPVDPP**, **TFPDPP, DTFPDPP** and **F3PDPP** calculated at the level of theory GGA-PW91/dnp using DMol[3].