**Spectroscopic Studies of the Optical, Thermal and Morphological Properties of a Newly Synthesized Self-Assembled PTCDI**

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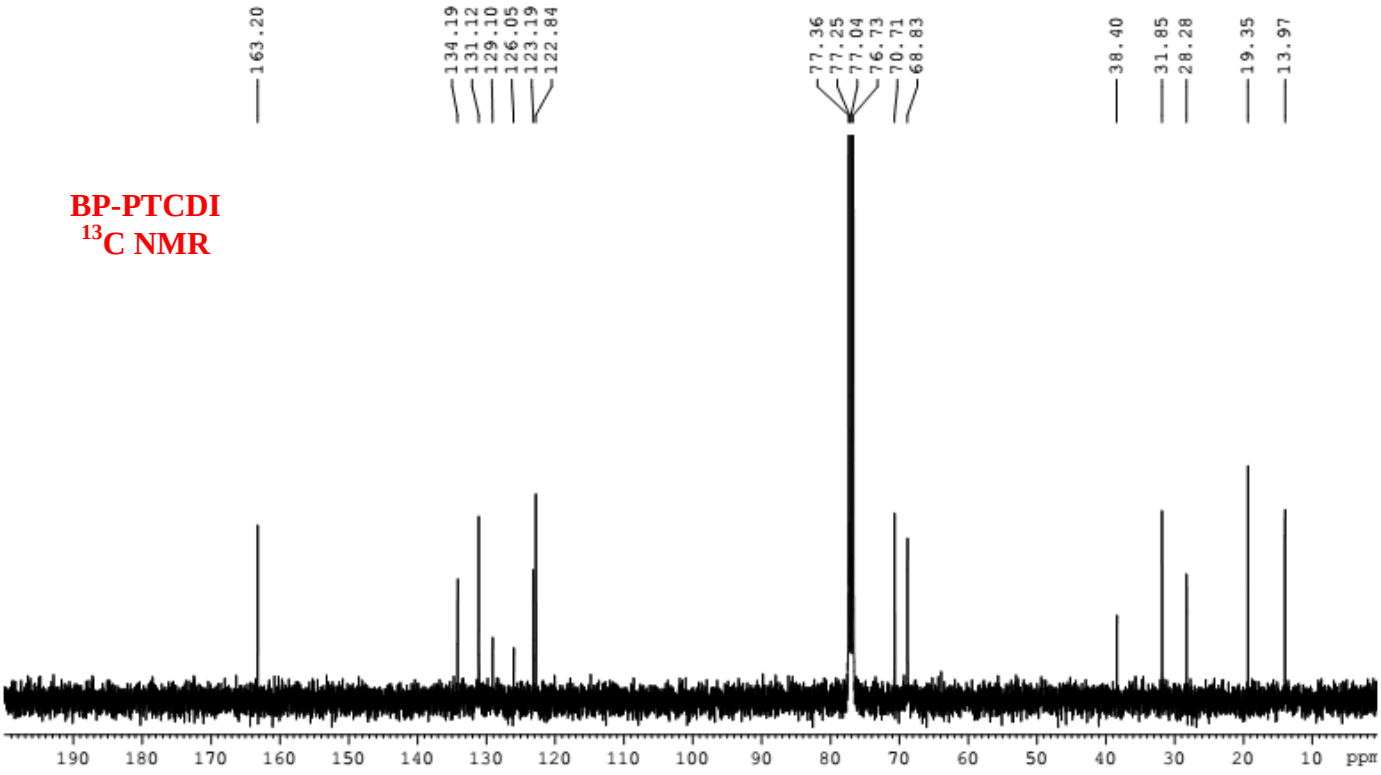

BP-PTCDI
13C NMR
163.20
134.19
131.12
129.10
126.05
123.19
122.84
77.36
77.25
77.04
76.73
70.71
68.83
38.40
31.85
28.28
19.35
13.97
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Fig S1

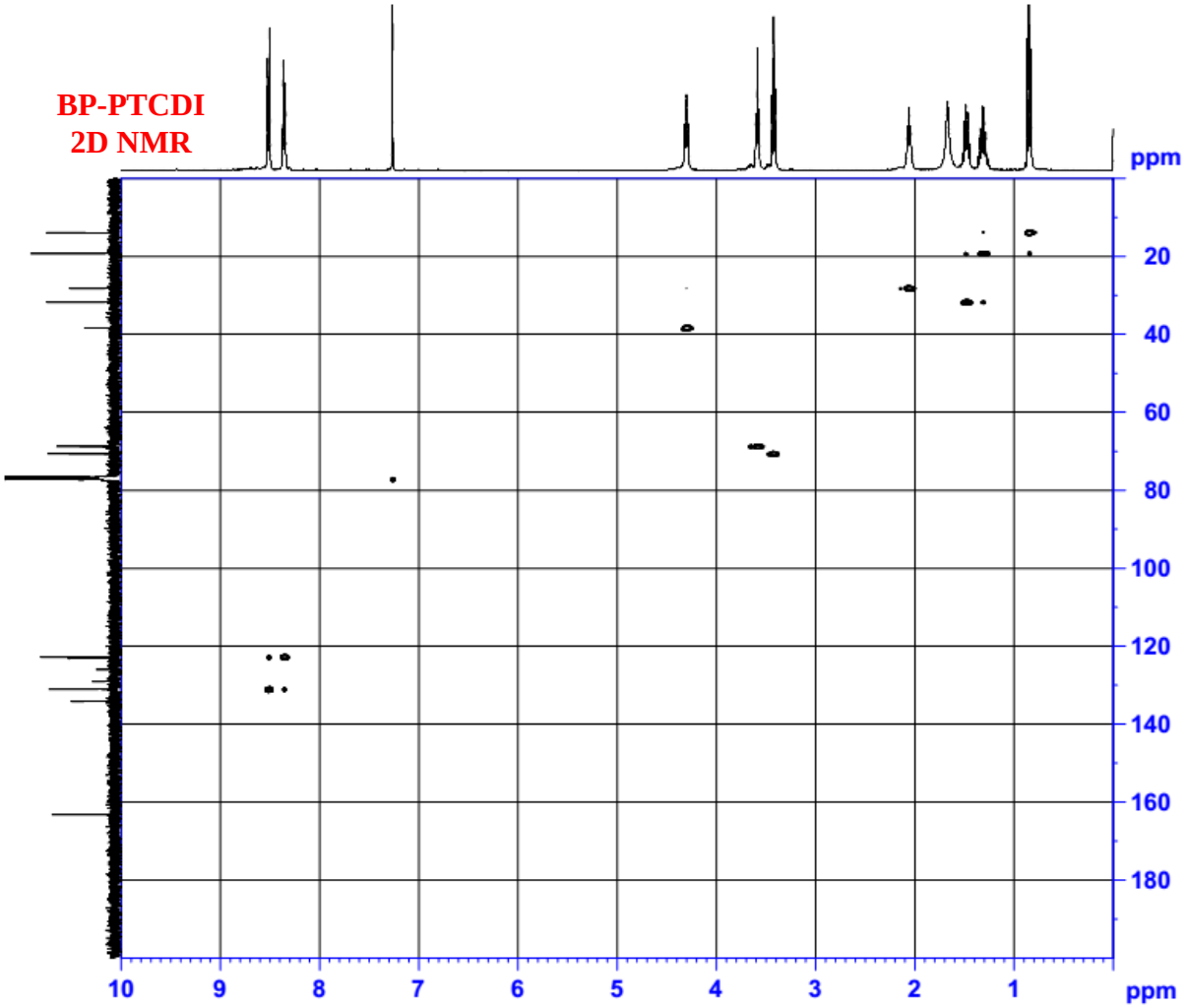

BP-PTCDI
2D NMR
ppm
20
40
60
80
100
120
140
160
180
10 9 8 7 6 5 4 3 2 1 ppm

Fig S2

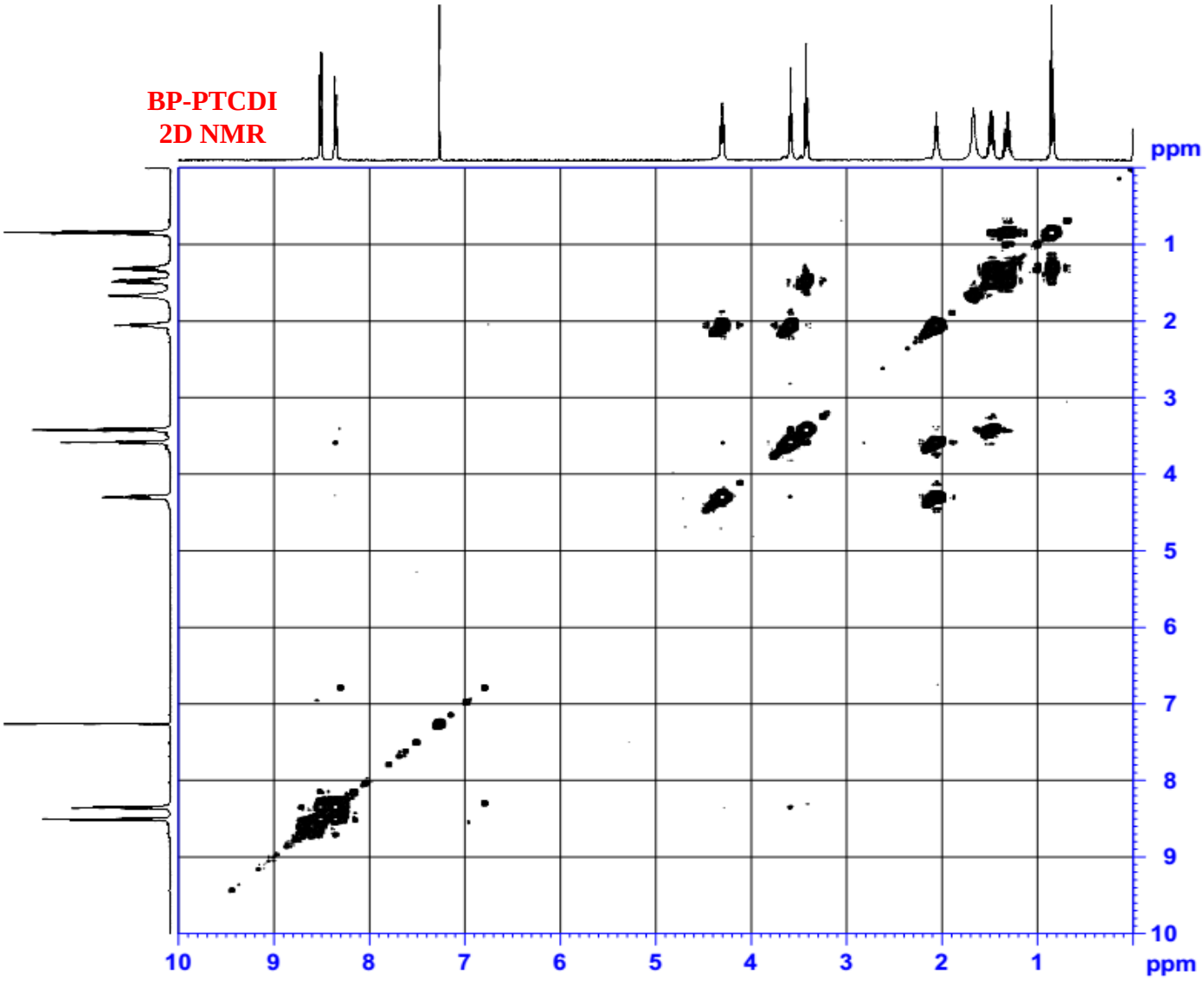
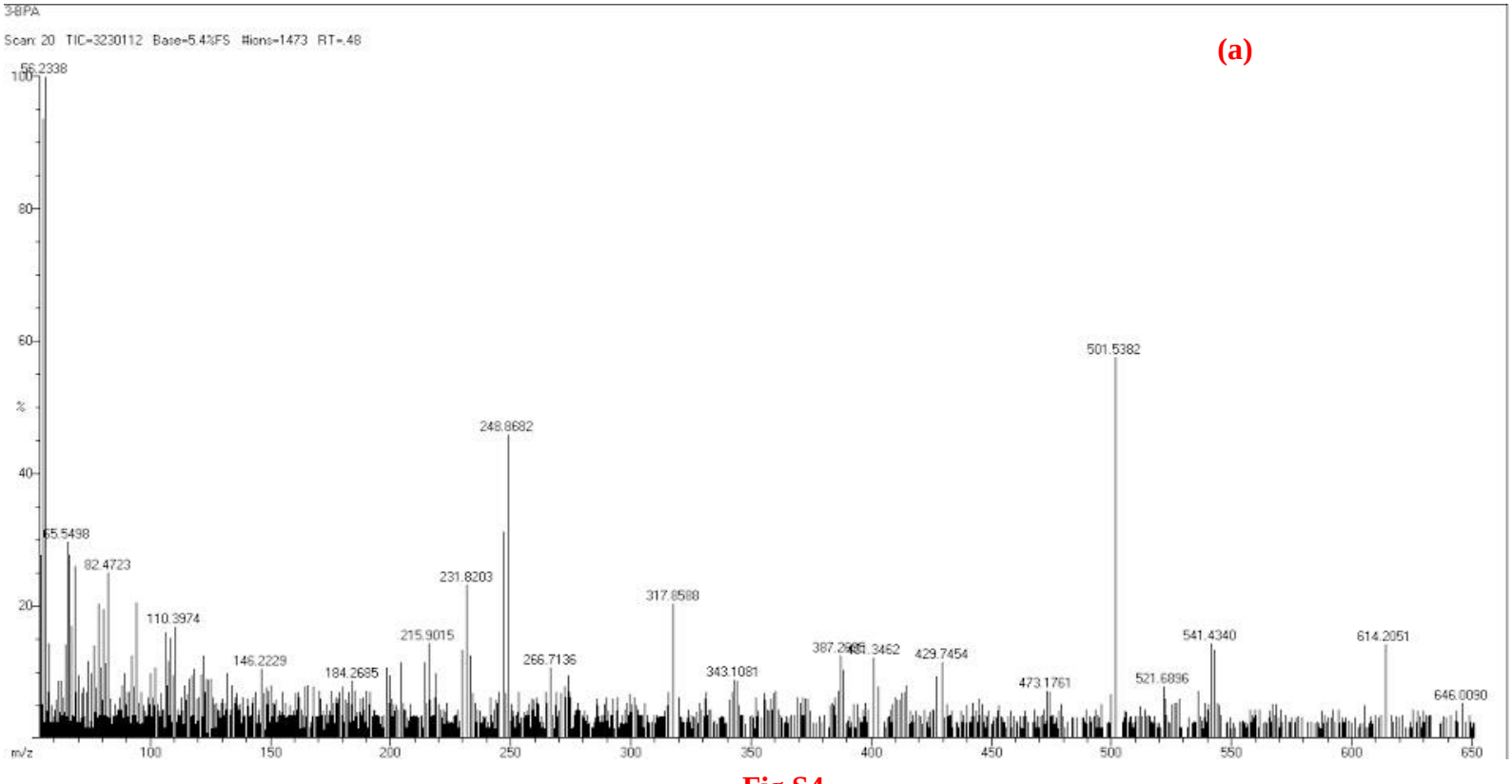

BP-PTCDI
2D NMR
ppm
1
2
3
4
5
6
7
8
9
10
10
9
8
7
6
5
4
3
2
1
ppm

Fig S3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Scan: 20 TIC=3230112 Base=5.4%FS #Ions=1473 RT=.48
(a)
56.2338
65.5498
82.4723
110.3974
146.2229
184.2685
215.9015
231.8203
248.8682
266.7136
317.8588
343.1081
387.2685
401.3462
429.7454
473.1761
501.5382
521.6896
541.4340
614.2051
646.0090
%
m/z

Fig S4

NBO table for compound BP-PTCDI

**Table 1**. Second order perturbation theory analysis of Fock matrix in NBO basis for BP

| | Donor (i) | ED(i)(e) | Acceptor (j) | ED(j)(e) | $E^{(2)}$kJ mol | E(j)-E(i) a.u | F(i,j)a.u |
|---|---|---|---|---|---|---|---|
| 1 | σ (C1-C2) | 1.97418 | π ( C3) | 0.00458 | 1.51 | 2.2 | 0.052 |
| 2 | | | σ ( C6) | 0.0045 | 0.77 | 2.03 | 0.035 |
| 3 | π (C1-C2) | 1.6521 | π ( C3 - C4) | 0.45293 | 20.45 | 0.28 | 0.07 |
| 4 | | | π ( C5 - C6) | 0.32243 | 17.65 | 0.29 | 0.064 |
| 5 | | | π ( C21 - O29) | 0.28979 | 22.35 | 0.27 | 0.071 |
| 6 | σ (C1-C6) | 1.97877 | π ( C5) | 0.00476 | 0.56 | 2.15 | 0.031 |
| 7 | σ (C2-C3) | 1.9691 | σ ( C1) | 0.00546 | 0.73 | 1.98 | 0.034 |
| 8 | π (C3-C4) | 1.52821 | π ( C1 - C2) | 0.30904 | 16.12 | 0.28 | 0.063 |
| 9 | | | π ( C5 - C6) | 0.32243 | 18.18 | 0.27 | 0.066 |
| 10 | | | π ( C7 - C8) | 0.30904 | 16.12 | 0.28 | 0.063 |
| 11 | | | π ( C9 - C10) | 0.32243 | 18.18 | 0.27 | 0.066 |
| 12 | π (C5-C6) | 1.64499 | π (C1-C2) | 0.30904 | 20.48 | 0.29 | 0.07 |
| 13 | | | π ( C3 - C4) | 0.45293 | 16.38 | 0.28 | 0.062 |
| 14 | | | π ( C11 - C20) | 0.32243 | 13.97 | 0.29 | 0.057 |
| 15 | σ ( C5 - C11) | 1.97121 | σ ( C4) | 0.00503 | 0.84 | 2.16 | 0.038 |
| 16 | | | π ( C4) | 0.00465 | 0.87 | 2.16 | 0.039 |
| 17 | | | σ ( C6) | 0.0045 | 1.15 | 1.99 | 0.043 |
| 18 | | | σ ( C17) | 0.00503 | 0.84 | 2.16 | 0.038 |
| 19 | | | π ( C17) | 0.00465 | 0.87 | 2.16 | 0.039 |
| 20 | π (C7-C8) | 1.6521 | π (C3-C4) | 0.45293 | 20.45 | 0.28 | 0.07 |
| 21 | | | π (C9-C10) | 0.32243 | 17.65 | 0.29 | 0.064 |
| 22 | | | π ( C23 - O30) | 0.28979 | 22.35 | 0.27 | 0.071 |
| 23 | σ ( C21 - O29) | 1.9942 | π ( C2) | 0.0047 | 0.84 | 2.31 | 0.039 |
| 24 | | | σ ( C21) | 0.01715 | 1.49 | 1.92 | 0.048 |
| 25 | | | π ( N22) | 0.00276 | 0.5 | 2.64 | 0.033 |
| 26 | σ ( N22) | 1.60066 | π ( C21 - O29 | 0.28979 | 54.95 | 0.27 | 0.111 |
| 27 | | | π ( C23 - O30) | 0.28979 | 54.95 | 0.27 | 0.111 |
| 28 | σ ( N25) | 1.60066 | π ( C24 - O28) | 0.28979 | 54.95 | 0.27 | 0.111 |
| 29 | | | π ( C26 - O27) | 0.28979 | 54.95 | 0.27 | 0.111 |
| 30 | σ ( O27) | 1.97704 | σ ( C26) | 0.01715 | 14.94 | 1.54 | 0.136 |
| 31 | | | σ ( C18 - C26) | 0.06348 | 2.48 | 1.12 | 0.048 |
| 32 | | | σ ( N25 - C 26) | 0.0872 | 1.57 | 1.1 | 0.038 |
| 33 | π ( O27) | 1.86307 | π ( C 26 | 0.0073 | 0.89 | 1.5 | 0.034 |
| 34 | | | σ ( C 18 - C 26 | 0.06348 | 18.81 | 0.69 | 0.104 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 35 | | | σ ( N25 - C26) | 0.0872 | 27.56 | 0.67 | 0.123 |
| 36 | σ ( O28) | 1.97704 | σ ( C24) | 0.01715 | 14.94 | 1.54 | 0.136 |
| 37 | π ( O28) | 1.86307 | σ ( C15 - C24) | 0.06348 | 18.81 | 0.69 | 0.104 |
| 38 | | | σ ( C24 - N25 | 0.08721 | 27.56 | 0.67 | 0.123 |
| 39 | σ ( O29) | 1.97704 | σ ( C21) | 0.01715 | 14.94 | 1.54 | 0.136 |
| 40 | π ( O29) | 1.86307 | σ ( C2- C21) | 0.06348 | 18.81 | 0.69 | 0.104 |
| 41 | | | σ ( C21 - N22) | 0.08721 | 27.56 | 0.67 | 0.123 |
| 42 | σ ( O30) | 1.97704 | σ ( C23) | 0.01715 | 14.94 | 1.54 | 0.136 |

[a]ED is the occupation number.
[b]$E^{(2)}$ is the energy of hyperconjugative interactions.
[c]Energy difference between donor and acceptor *i* and *j* NBO orbitals.
[d]F(*i*,*j*) is the Fock matrix element between *i* and *j* NBO orbitals.