Electronic Supplementary Material (ESI) for CrystEngComm.

Exploration of relative π-electron localization in naphthalene aromatic ring by C–H···π interactions: experimental evidence, computational criteria, and database analysis

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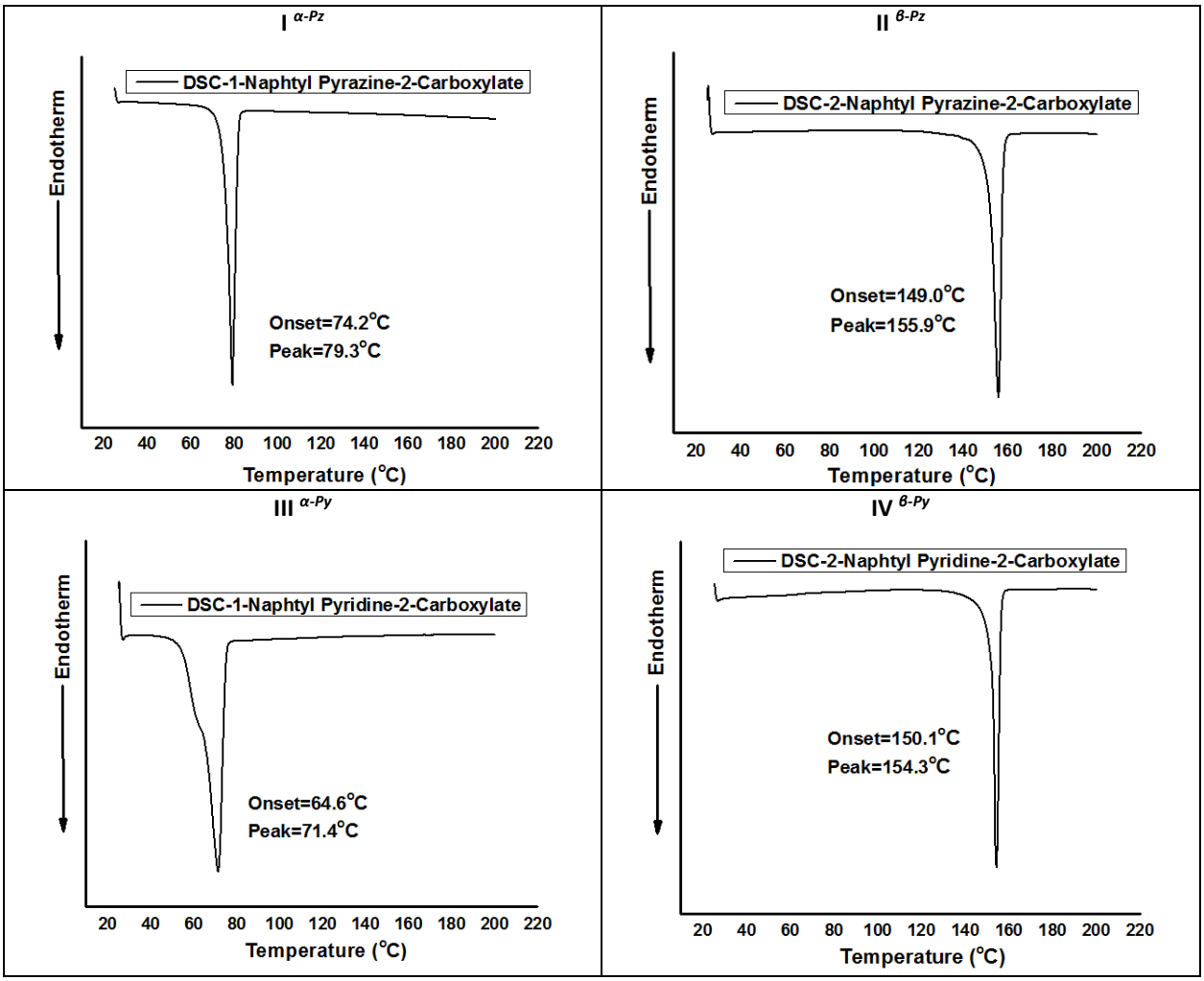
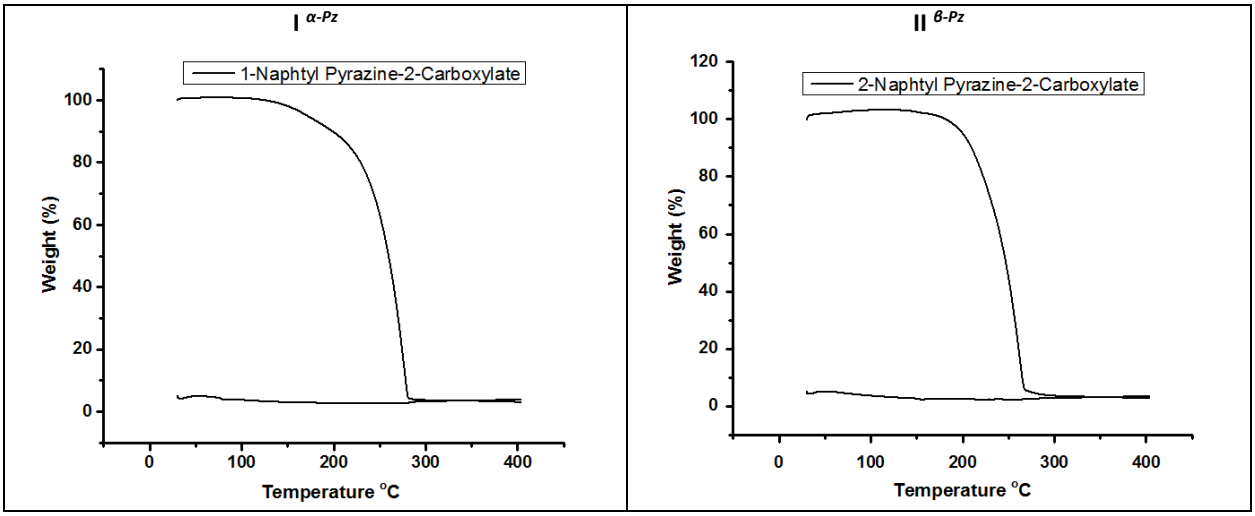
Supporting Information

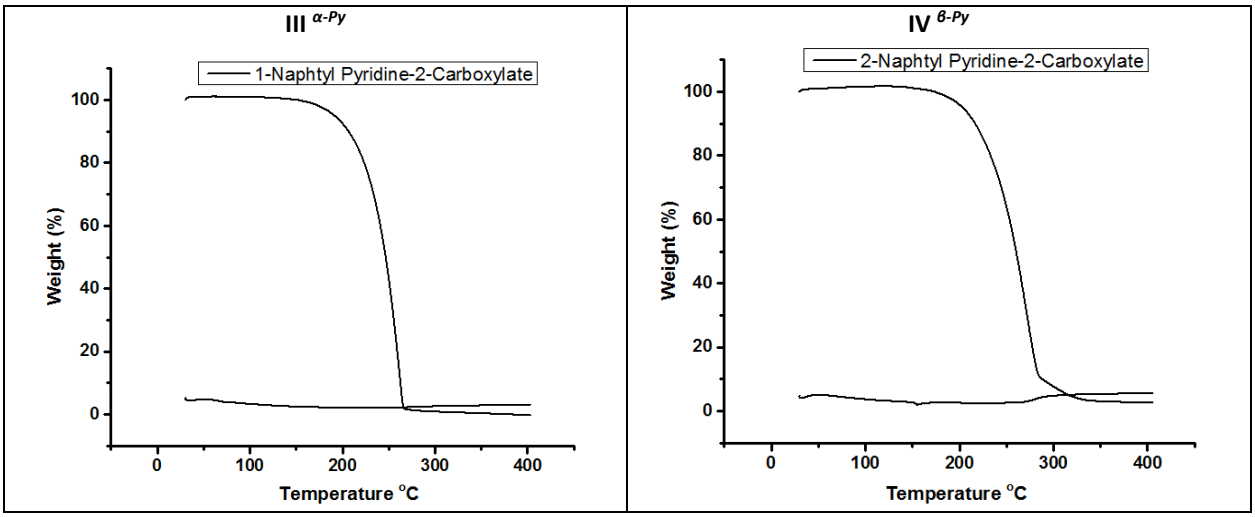
S0. List of Contents

S1. DSC diagrams for I $^{\alpha\text{-}Pz}$, II $^{\beta\text{-}Pz}$, III $^{\alpha\text{-}Py}$, IV $^{\beta\text{-}Py}$.

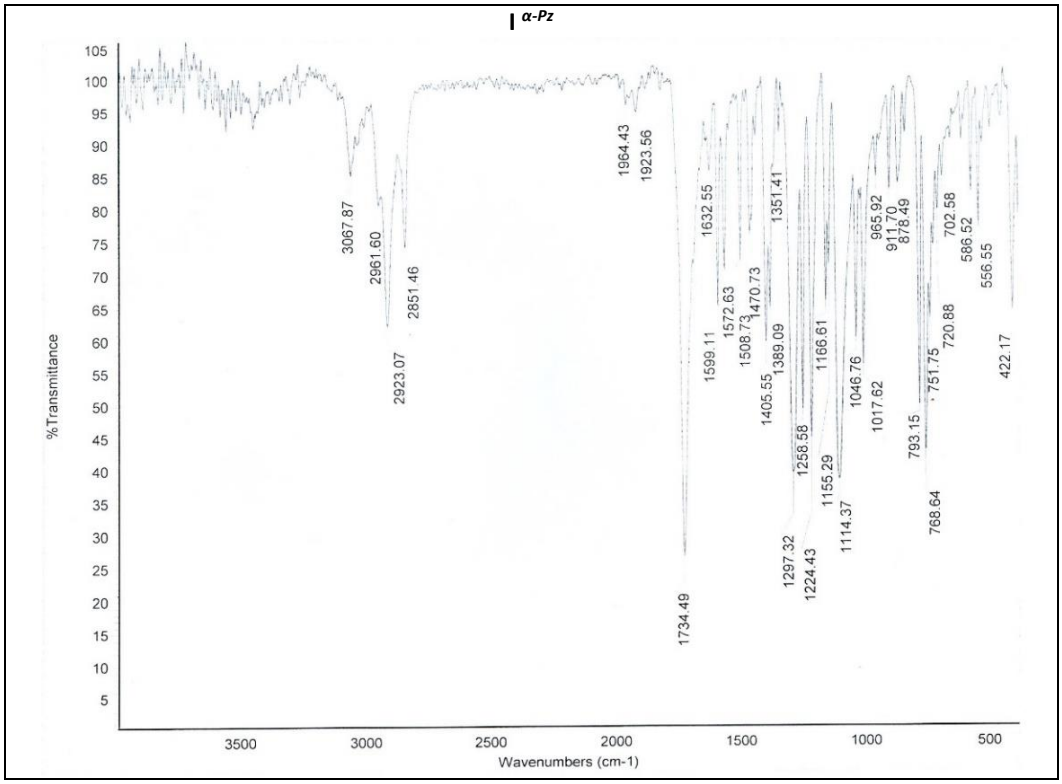


S2. TGA diagrams for I $^{\alpha\text{-}Pz}$, II $^{\beta\text{-}Pz}$, III $^{\alpha\text{-}Py}$, IV $^{\beta\text{-}Py}$.

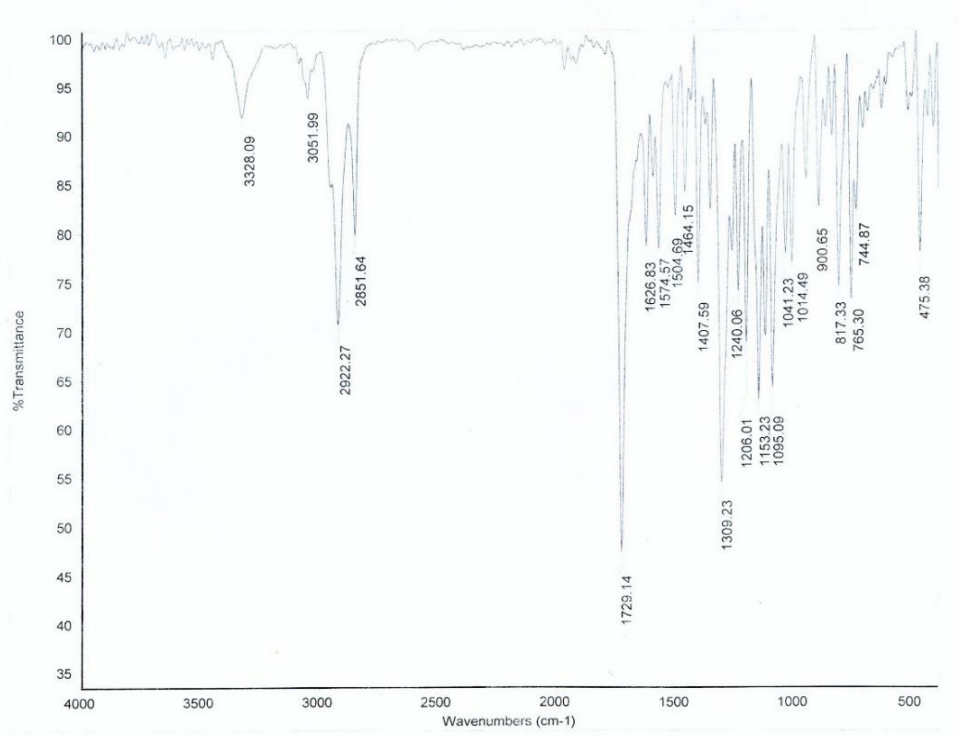




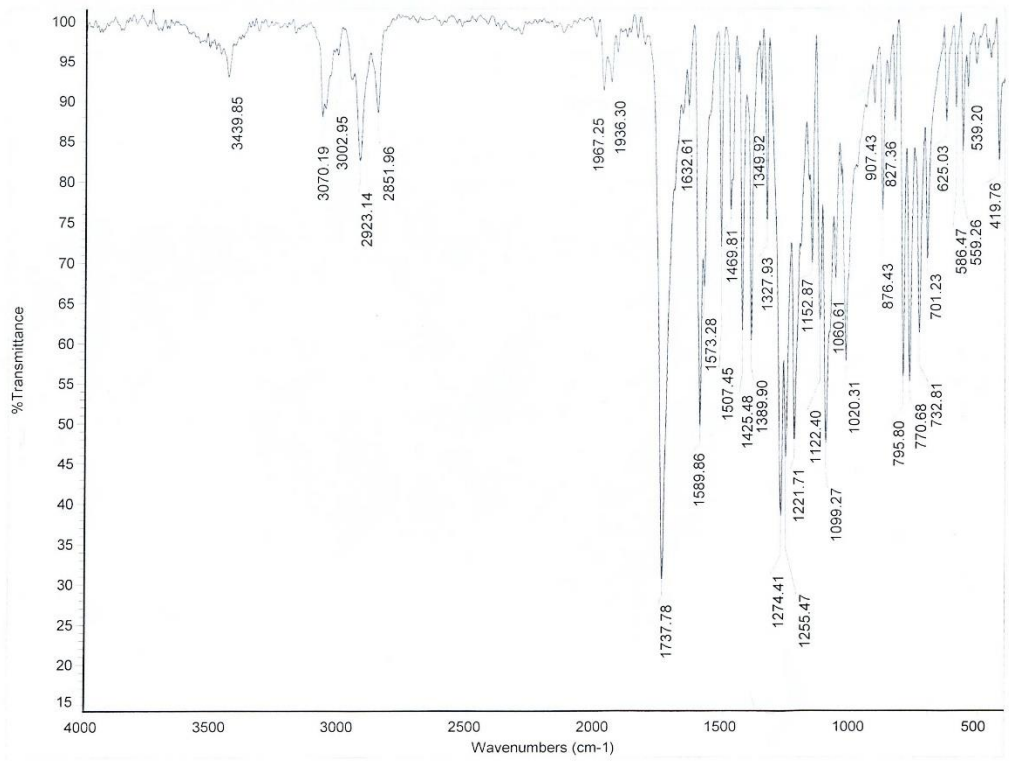
S3. FT-IR transmittance plots for I $^{\alpha\text{-}Pz}$, II $^{\beta\text{-}Pz}$, III $^{\alpha\text{-}Py}$, IV $^{\beta\text{-}Py}$.



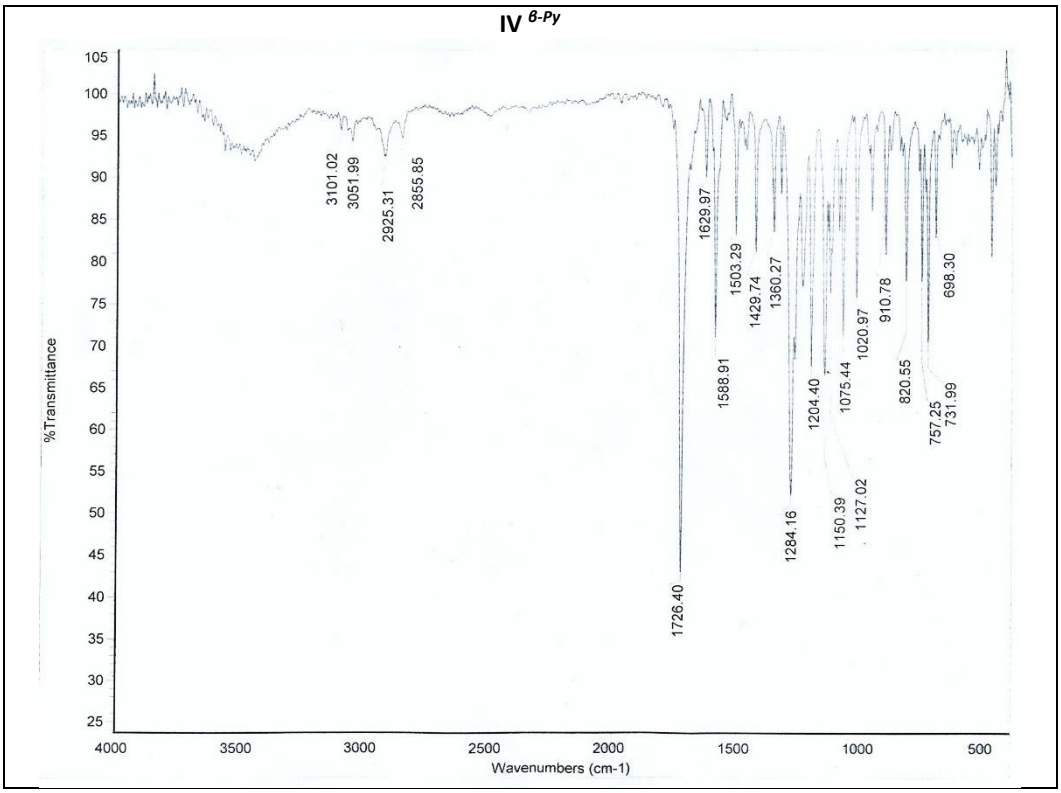
II ***β-Pz***



III ***α-Py***



IV ***β-Py***



S4. CHN-elemental analysis for I ***α-Pz***, II ***β-Pz***, III ***α-Py***, IV ***β-Py***.

I ***α-Pz***

Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-35		

#	Group	Sample Name	Type	Weig.	Pro.F		
35	1	AS3	UNK	1.024	6.25	---	

Component name	Element %
Nitrogen%	10.95125294
Carbon%	75.19926453
Hydrogen%	4.31277895
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	10.95125294
Carbon%	75.19926453
Hydrogen%	4.31277895
Sulphur%	0

II ***β-Pz***

Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-71		

#	Group	Sample Name	Type	Weig.	Pro.F		
71	1	AS1	UNK	0.939	6.25	---	

Component name	Element %
Nitrogen%	11.09747314
Carbon%	73.56679535
Hydrogen%	4.583220959
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	11.09747314
Carbon%	73.56679535
Hydrogen%	4.583220959
Sulphur%	0

III ***α-Py***

Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-34		

#	Group	Sample Name	Type	Weig.	Pro.F		
34	1	AS2	UNK	1.041	6.25	---	

Component name	Element %
Nitrogen%	5.501227379
Carbon%	79.83586884
Hydrogen%	4.67258215
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	5.501227379
Carbon%	79.83586884
Hydrogen%	4.67258215
Sulphur%	0

IV ***β-Py***

Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-72		

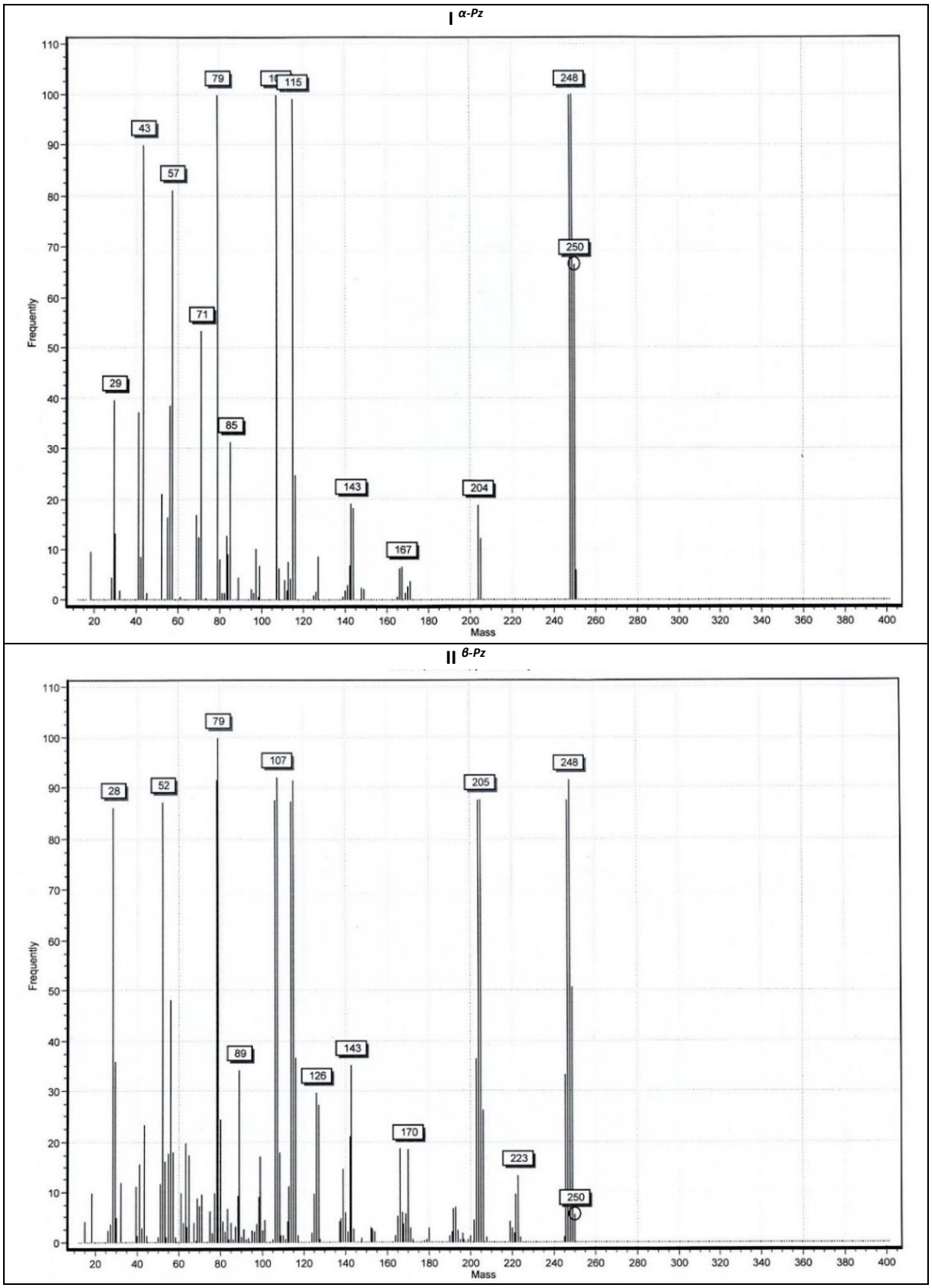
#	Group	Sample Name	Type	Weig.	Pro.F		
72	1	AS4	UNK	1.068	6.25	---	

Component name	Element %
Nitrogen%	5.741287231
Carbon%	78.52898407
Hydrogen%	4.847149372
Sulphur%	0

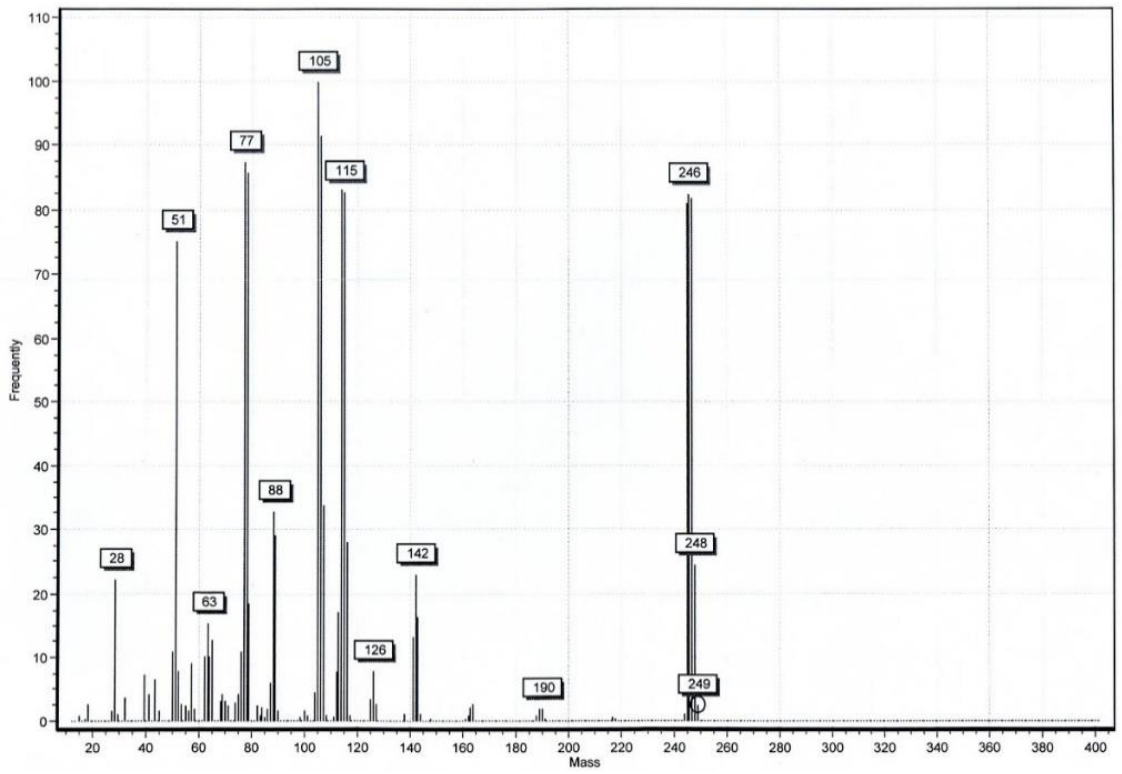
1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	5.741287231
Carbon%	78.52898407
Hydrogen%	4.847149372
Sulphur%	0

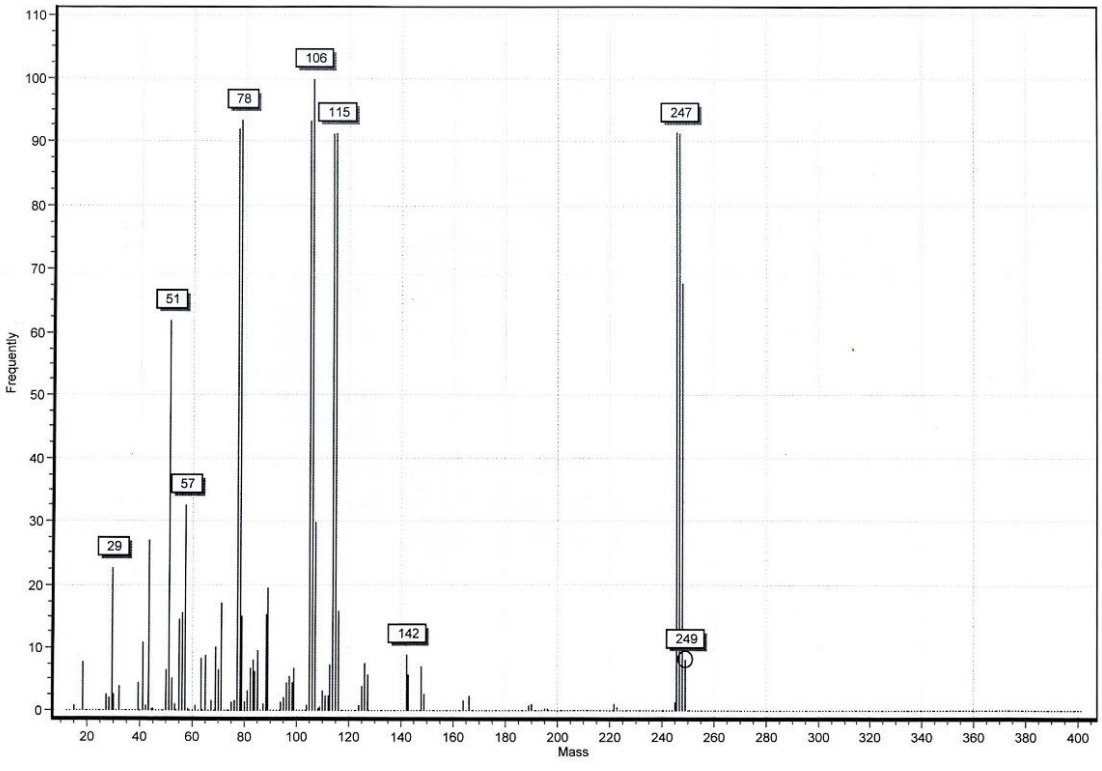
S5. Mass spectroscopy analysis for I $^{\alpha\text{-}Pz}$, II $^{\beta\text{-}Pz}$, III $^{\alpha\text{-}Py}$, IV $^{\beta\text{-}Py}$.



III ***α-Py***

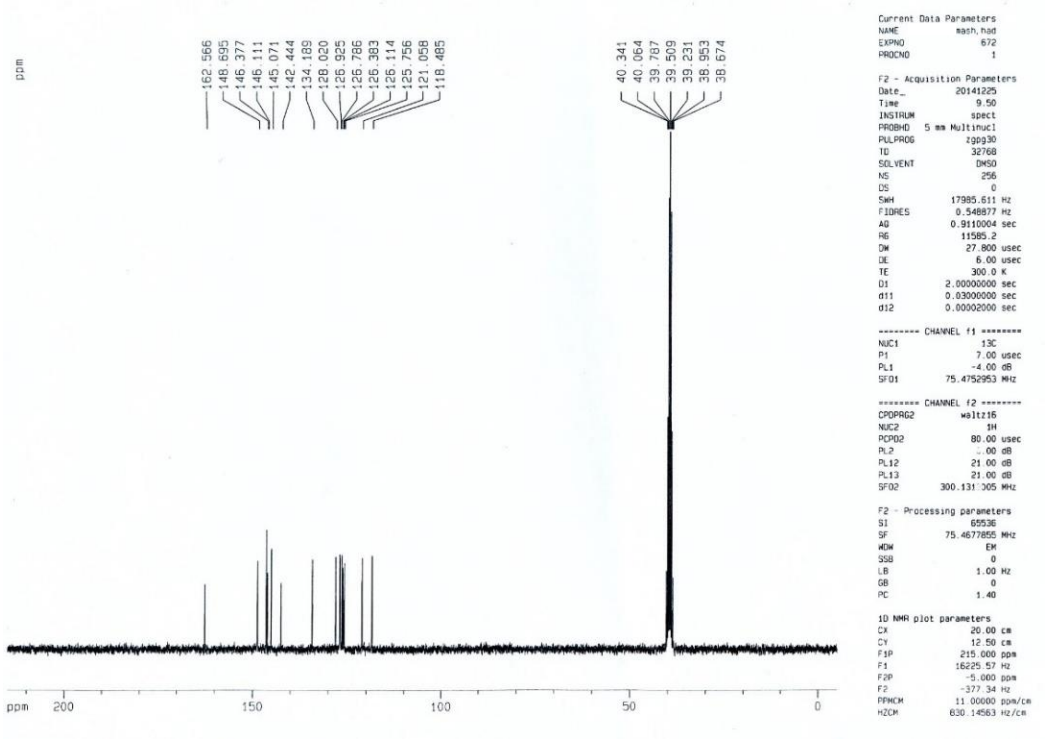


IV ***β-Py***

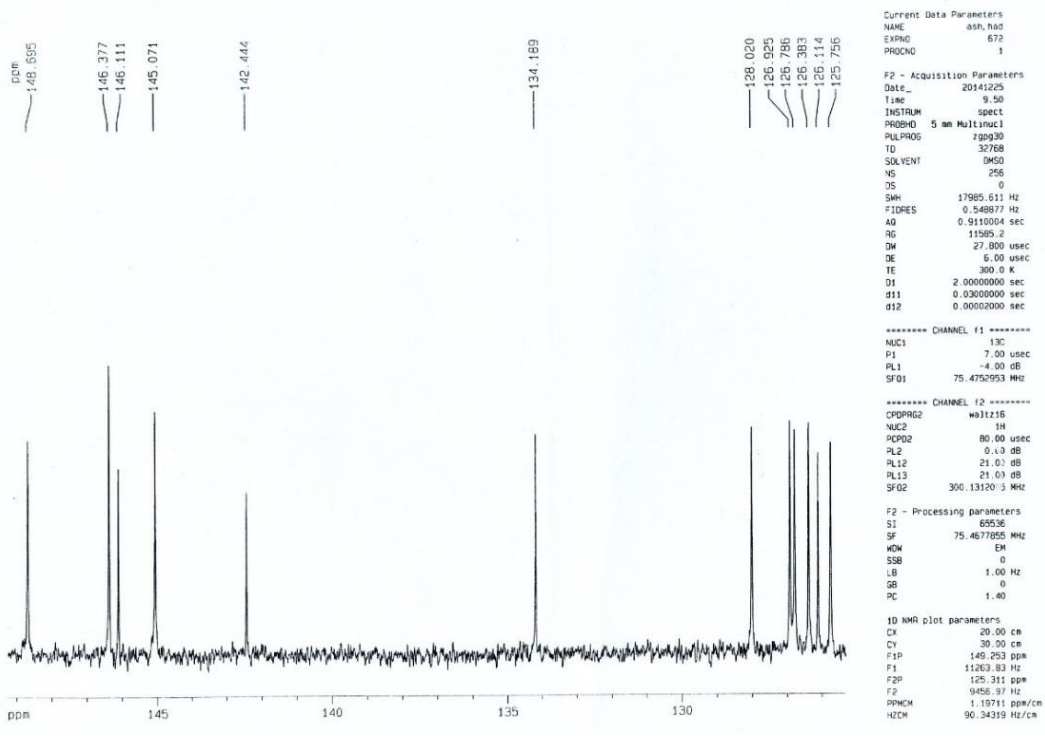


S6. ^{13}C-NMR spectra for I $^{\alpha\text{-}Pz}$, II $^{\beta\text{-}Pz}$, III $^{\alpha\text{-}Py}$, IV $^{\beta\text{-}Py}$.

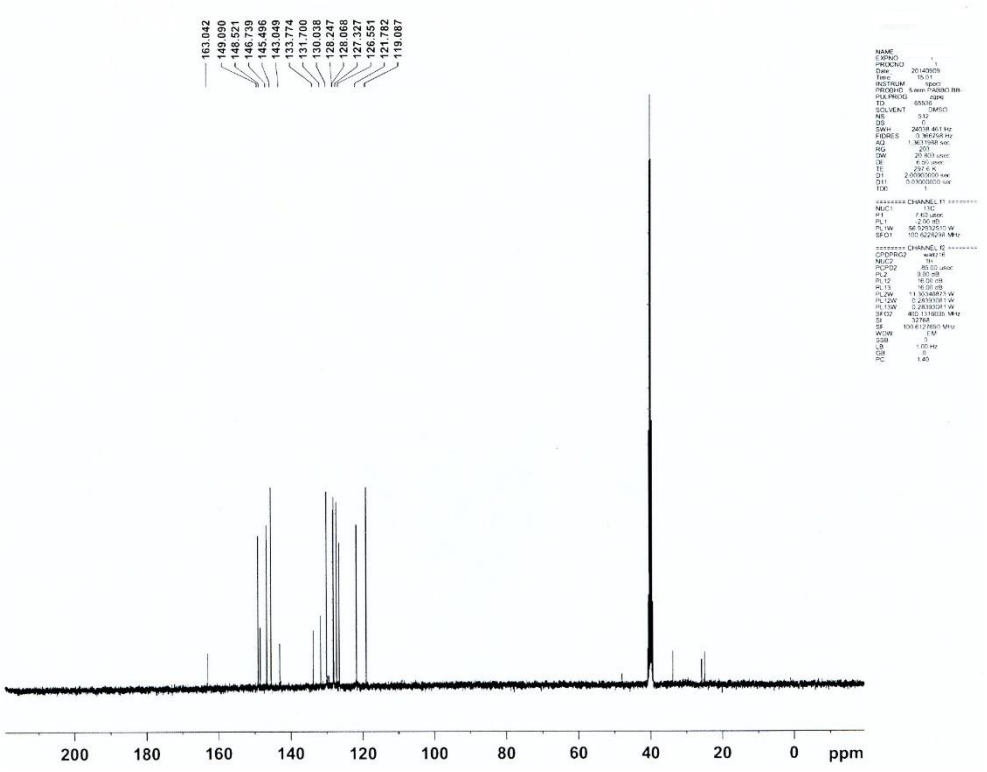
I $^{\alpha\text{-}Pz}$



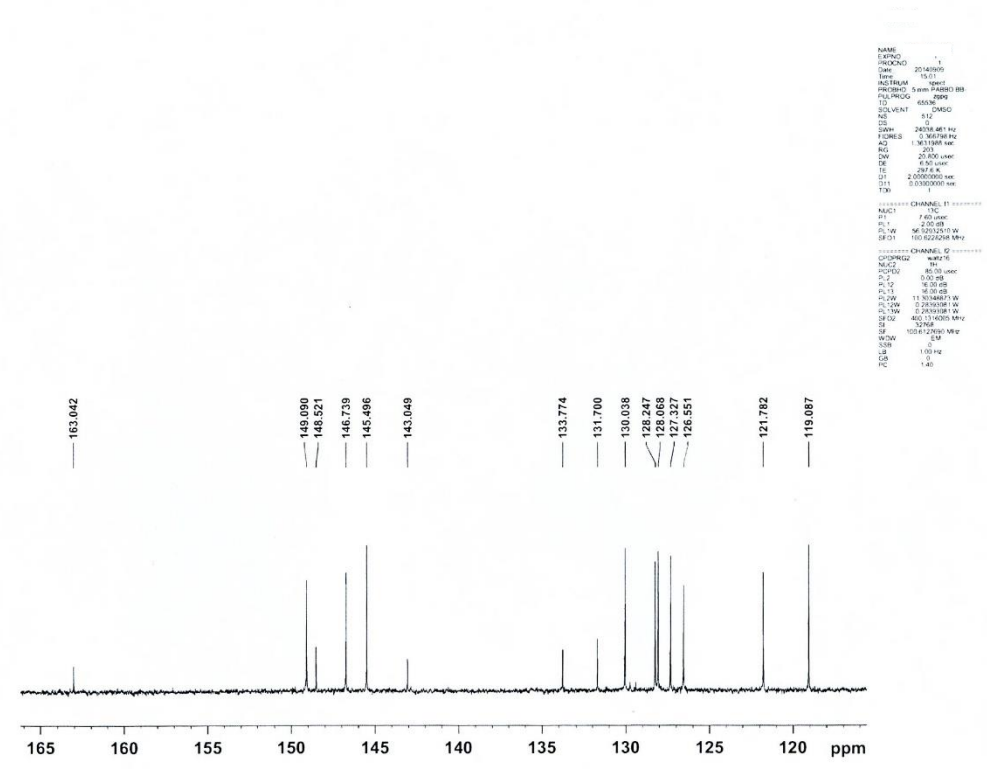
I $^{\alpha\text{-}Pz}$-Expansion



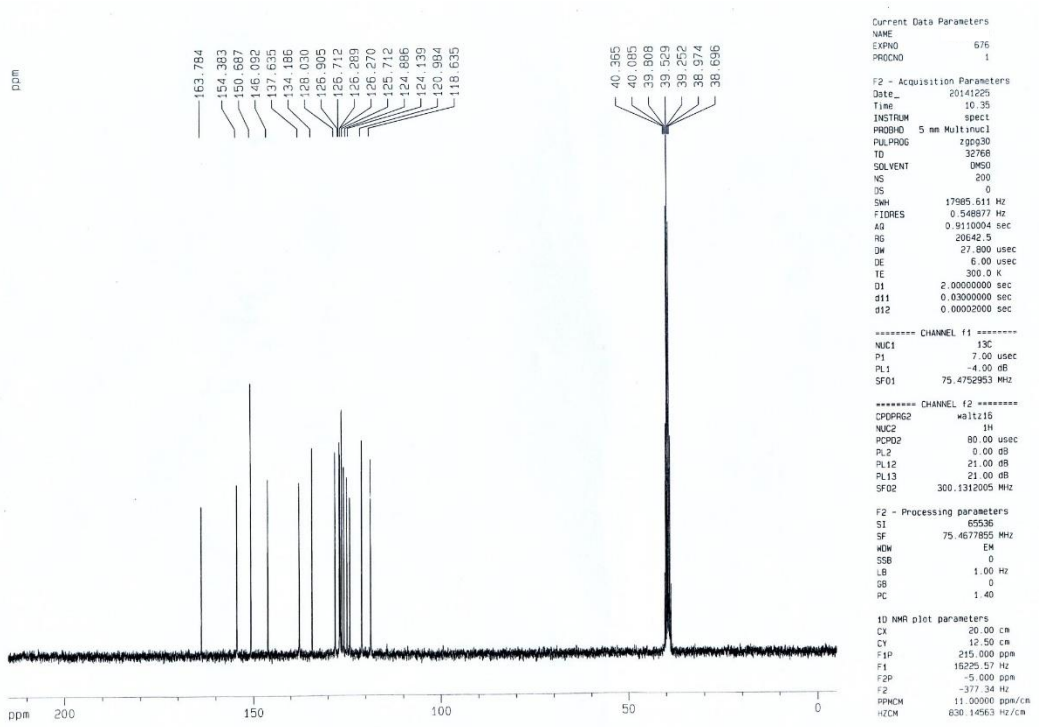
II ***β-Pz***



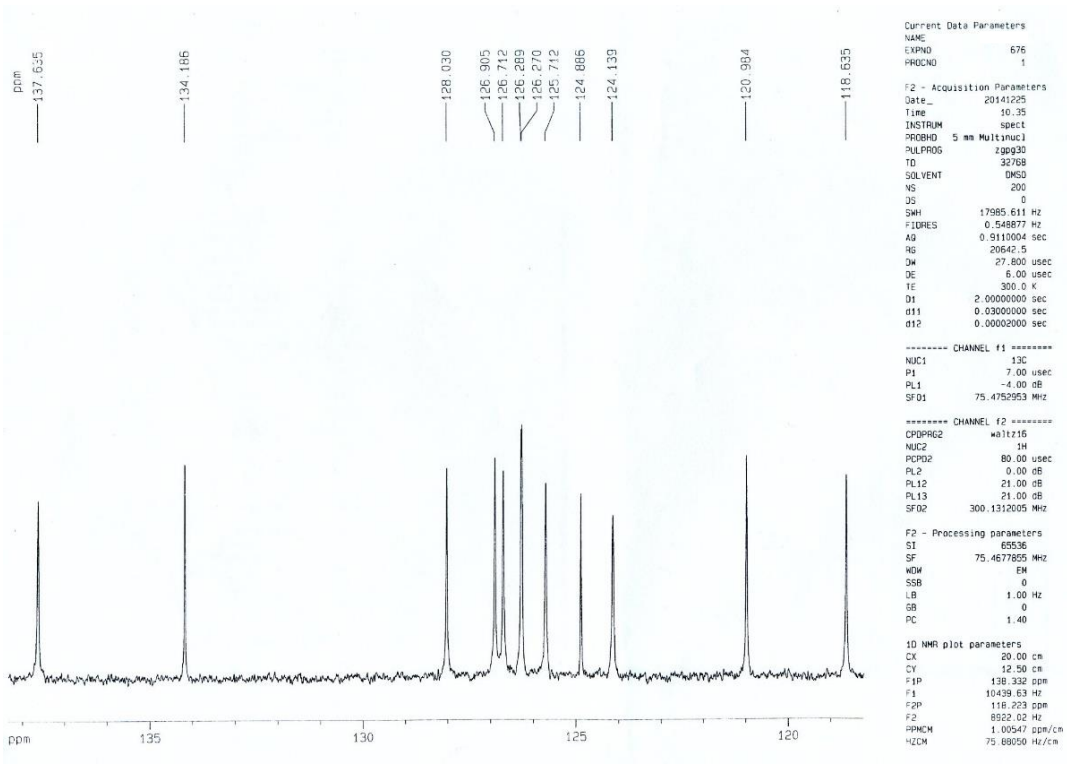
II ***β-Pz*****-Expansion**



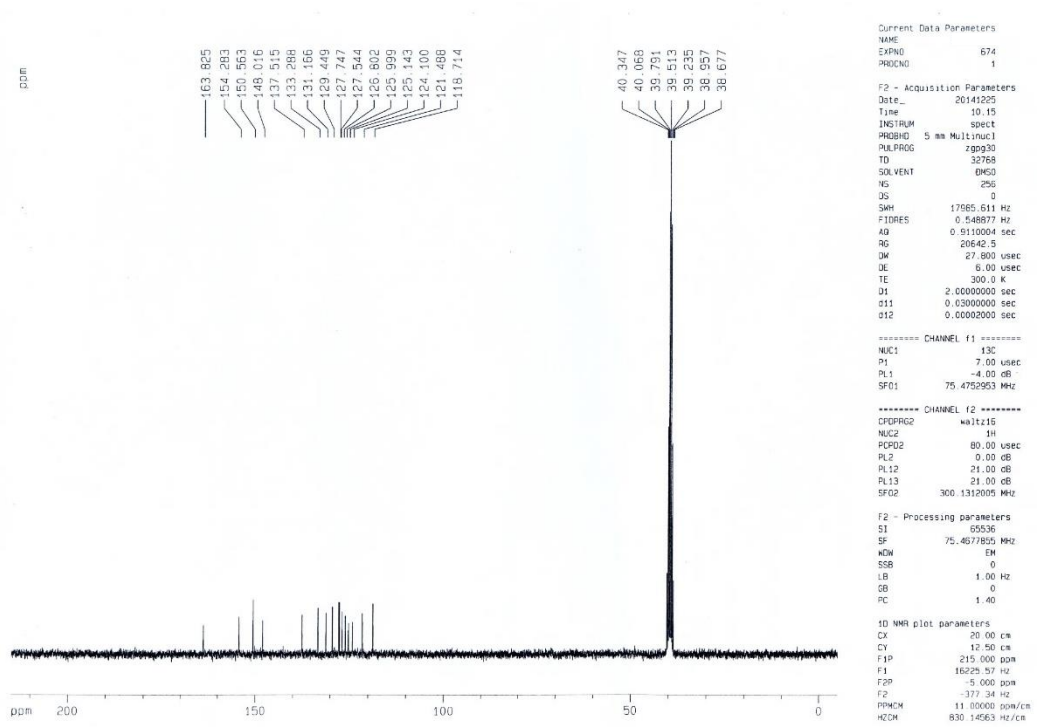
III $^{\alpha\text{-}Py}$



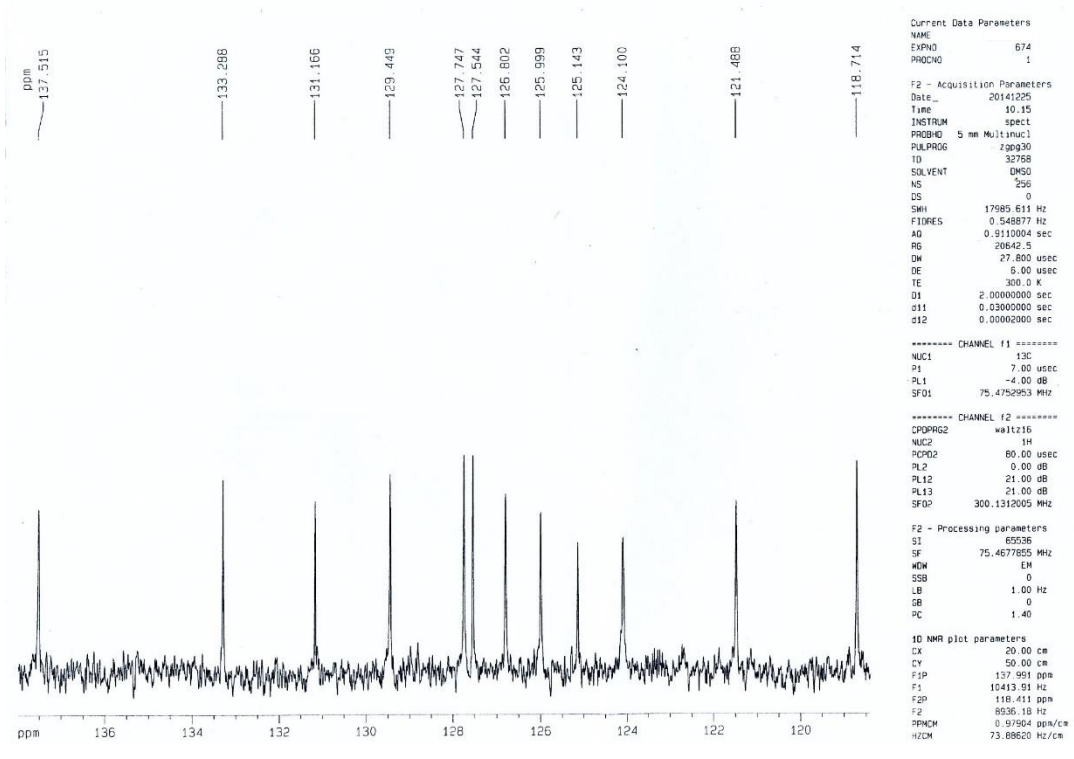
III $^{\alpha\text{-}Py}$-Expansion



IV *β-Py*

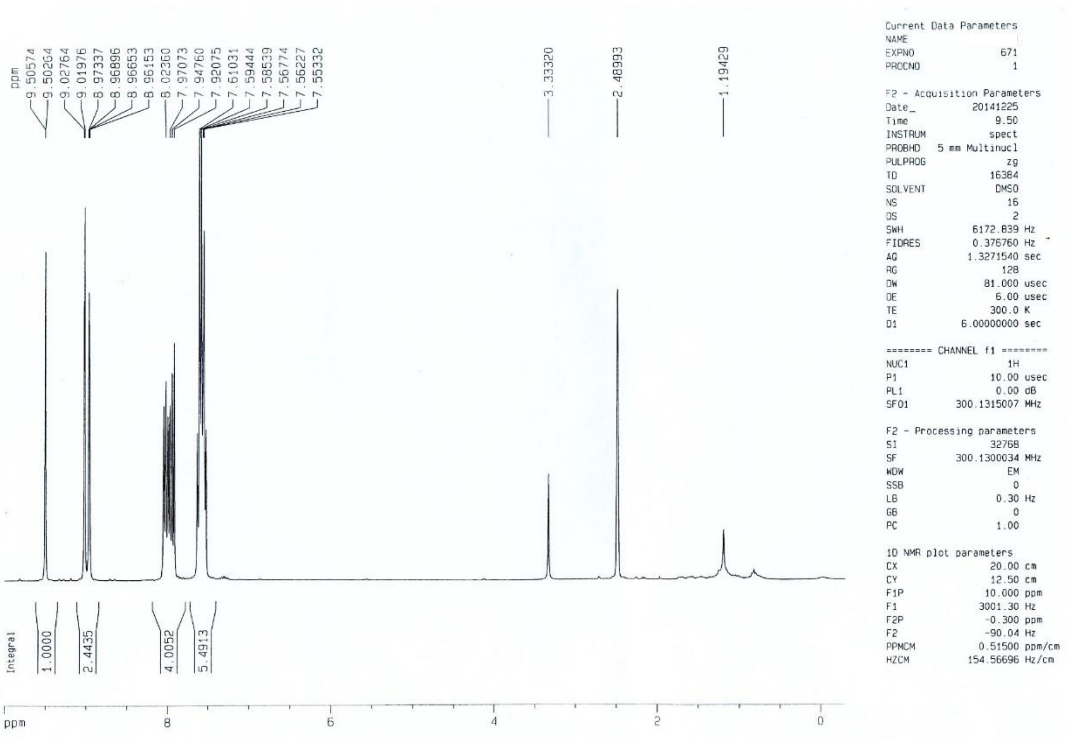


IV *β-Py*-Expansion

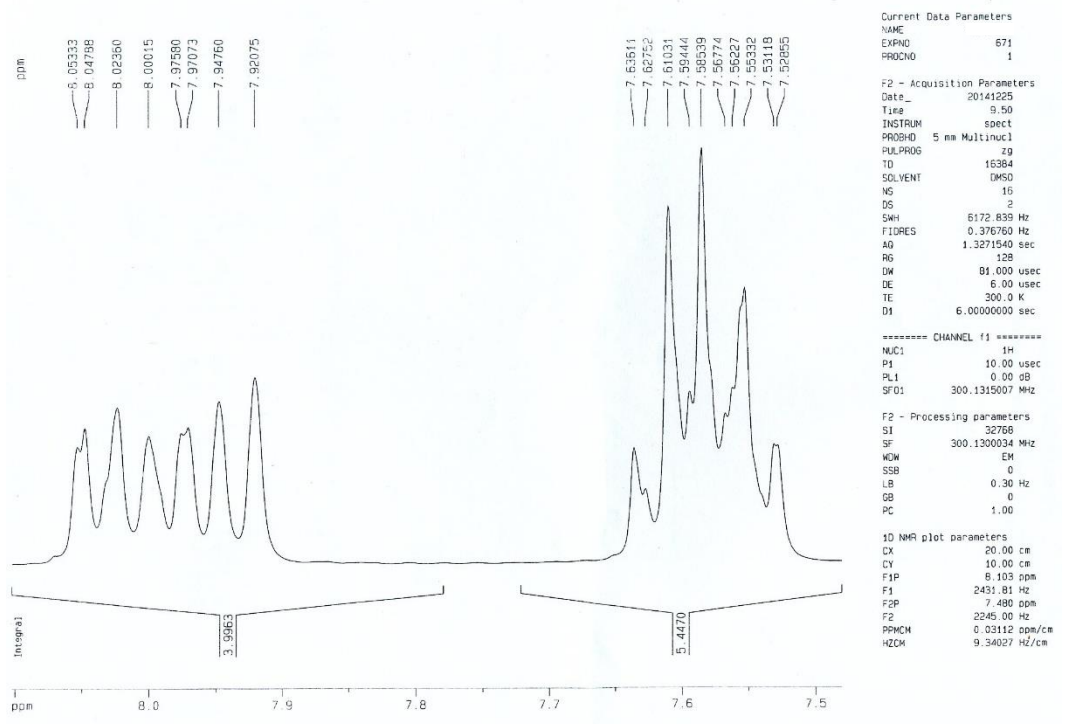


S7. ^{1}H-NMR spectra for I $^{\alpha\text{-}Pz}$, II $^{\beta\text{-}Pz}$, III $^{\alpha\text{-}Py}$, IV $^{\beta\text{-}Py}$.

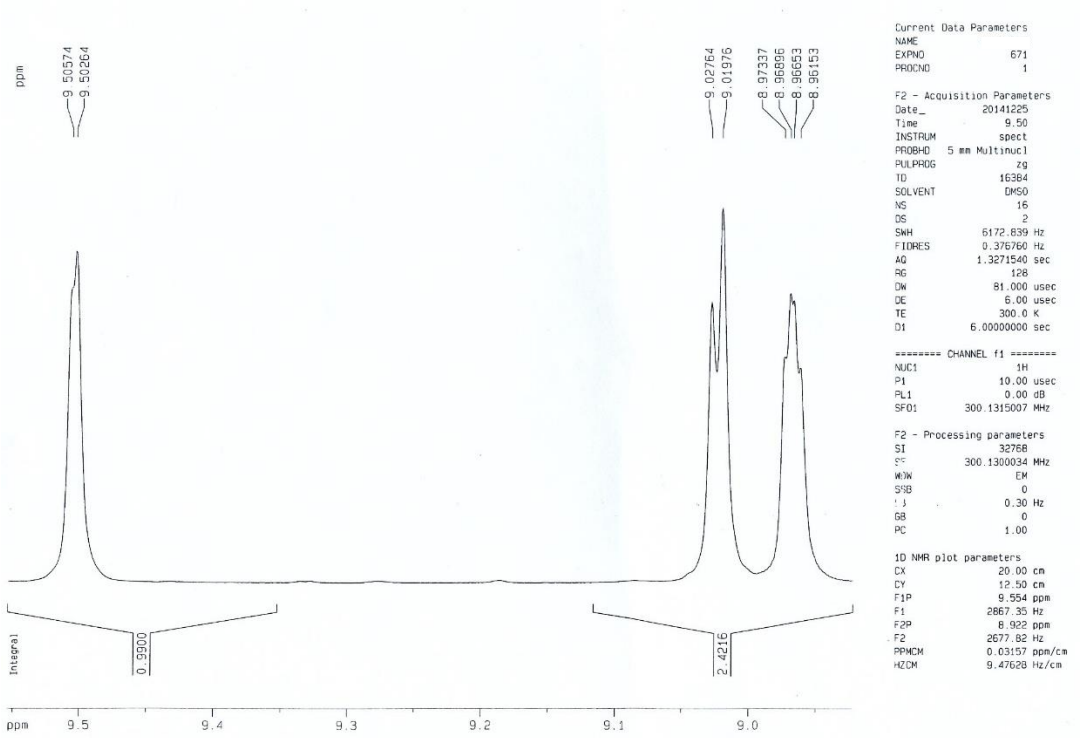
I $^{\alpha\text{-}Pz}$



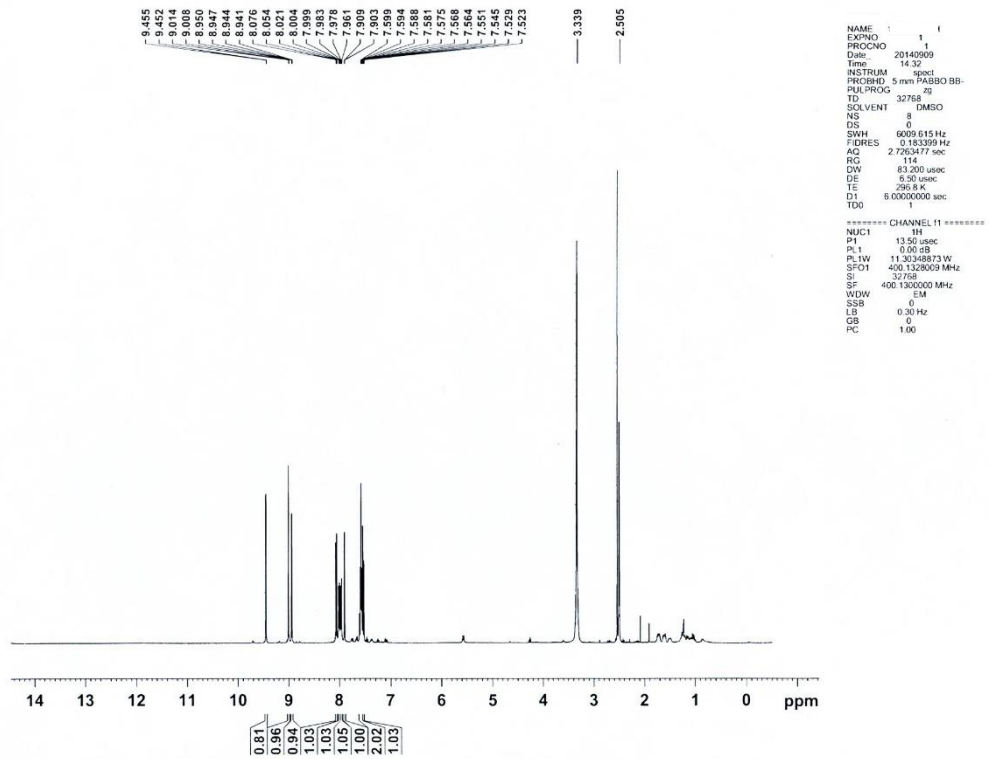
I $^{\alpha\text{-}Pz}$-Expansion



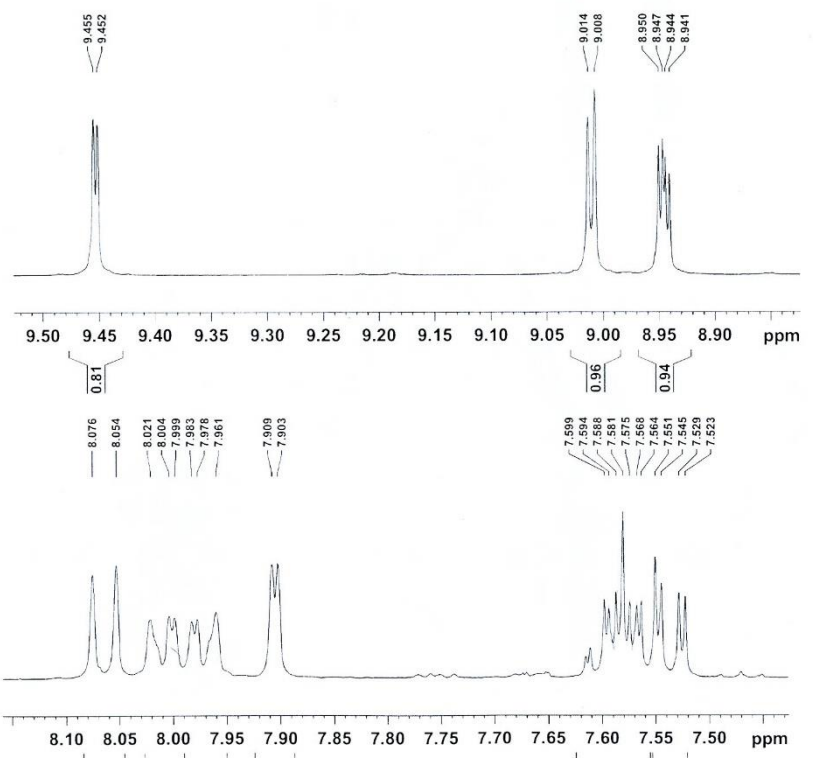
I $^{\alpha\text{-}Pz}$-Expansion



II $^{\beta\text{-}Pz}$



II $^{\beta\text{-}Pz}$ -Expansion

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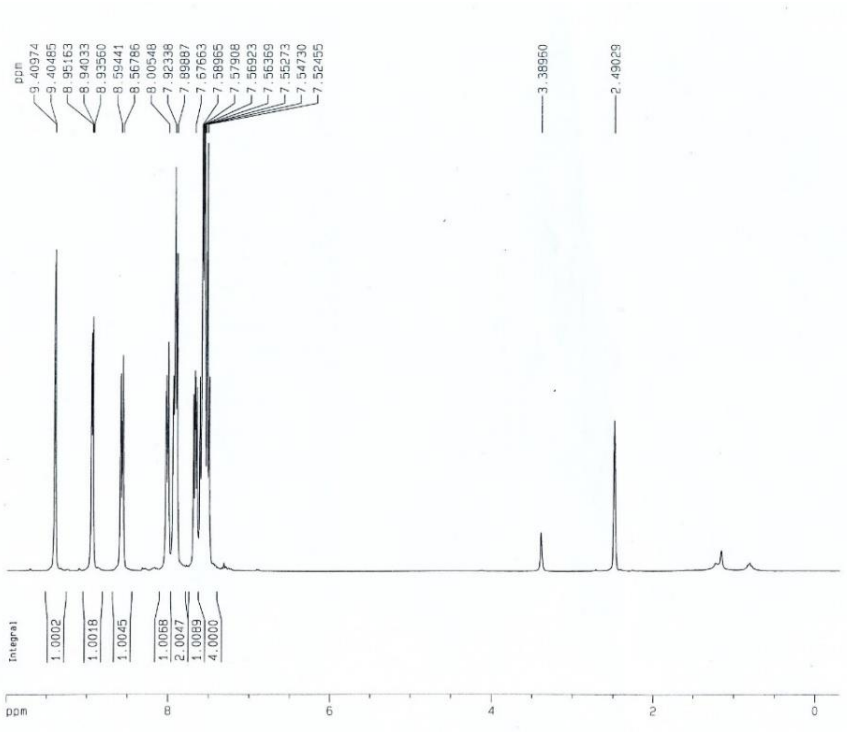
NAME
EXPNO          1
PROCNO         1
Date_       20140909
Time           14.32
INSTRUM         spect
PROBHD  5 mm PABBO BB-
PULPROG         zg
TD             32768
SOLVENT         DMSO
NS                 8
DS                 0
SWH         6009.615 Hz
FIDRES      0.183398 Hz
AQ          2.7263477 sec
RG               114
DW          83.200 usec
DE           6.50 usec
TE           296.8 K
D1          6.00000000 sec
TD0                1

======== CHANNEL f1 ====
NUC1             1H
P1           13.50 usec
PL1           0.00 dB
PL1W     11.30348873 W
SFO1     400.1328009 MHz
SI             32768
SF       400.1300000 MHz
WDW              EM
SSB               0
LB             0.30 Hz
GB                0
PC             1.00
```

III $^{\alpha\text{-}Py}$

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Current Data Parameters
NAME
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PROCNO                 1

F2 - Acquisition Parameters
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Time               10.27
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG               zg
TD                 16384
SOLVENT             DMSO
NS                    16
DS                     2
SWH             6172.839 Hz
FIDRES          0.376760 Hz
AQ              1.3271540 sec
RG                  50.8
DW              81.000 usec
DE               6.00 usec
TE               300.0 K
D1          6.00000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1              10.00 usec
PL1              0.00 dB
SFO1        300.1315007 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300034 MHz
WDW                   EM
SSB                    0
LB              0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P               10.000 ppm
F1              3001.30 Hz
F2P               -0.300 ppm
F2               -90.04 Hz
PPMCM           0.51500 ppm/cm
HZCM          154.56696 Hz/cm
```
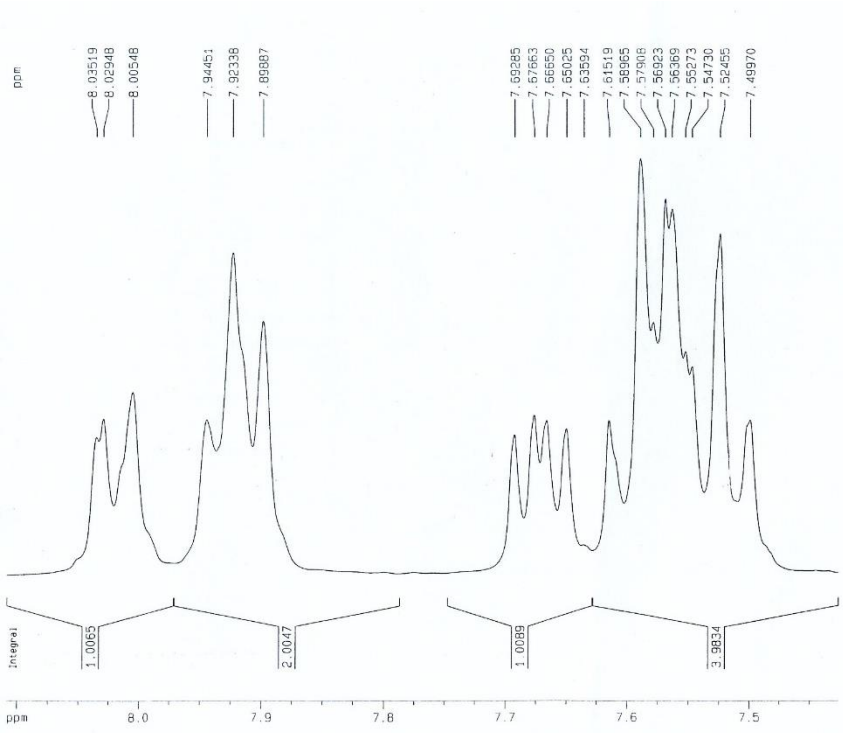

III $^{\alpha\text{-}Py}$-Expansion



Current Data Parameters
NAME
EXPNO 675
PROCNO 1

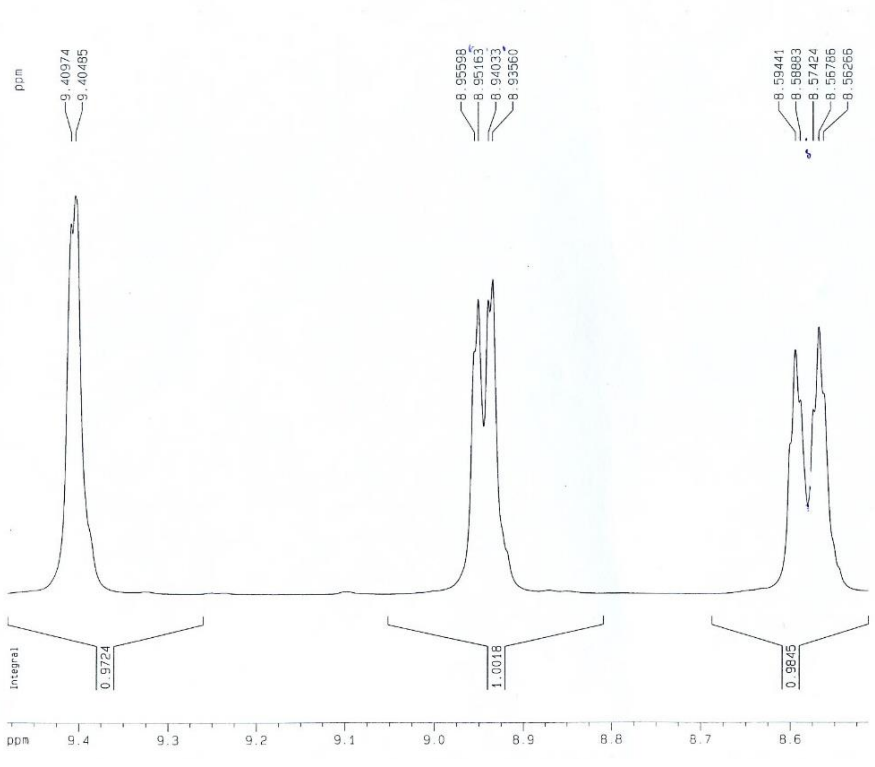
F2 - Acquisition Parameters
Date_ 20141225
Time 10.27
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg
TD 16384
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 50.8
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 8.108 ppm
F1 2433.52 Hz
F2P 7.426 ppm
F2 2228.85 Hz
PPMCM 0.03410 ppm/cm
HZCM 10.23358 Hz/cm

III $^{\alpha\text{-}Py}$-Expansion



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EXPNO 675
PROCNO 1

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Date_ 20141225
Time 10.27
INSTRUM spect
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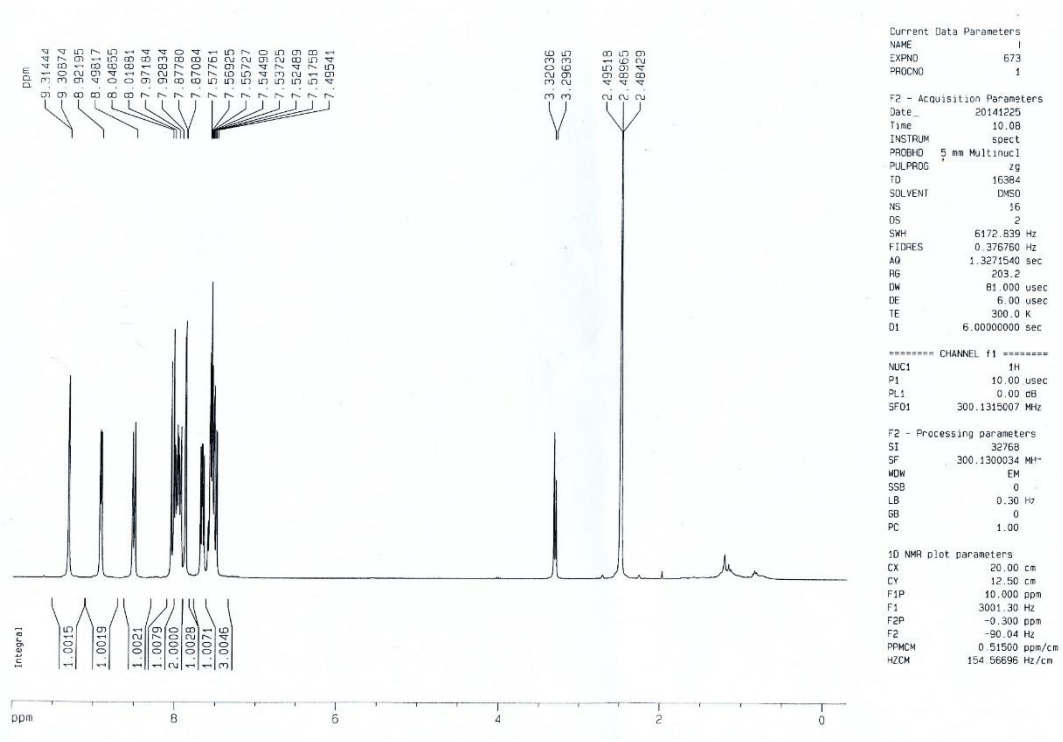
PULPROG zg
TD 16384
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 50.8
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

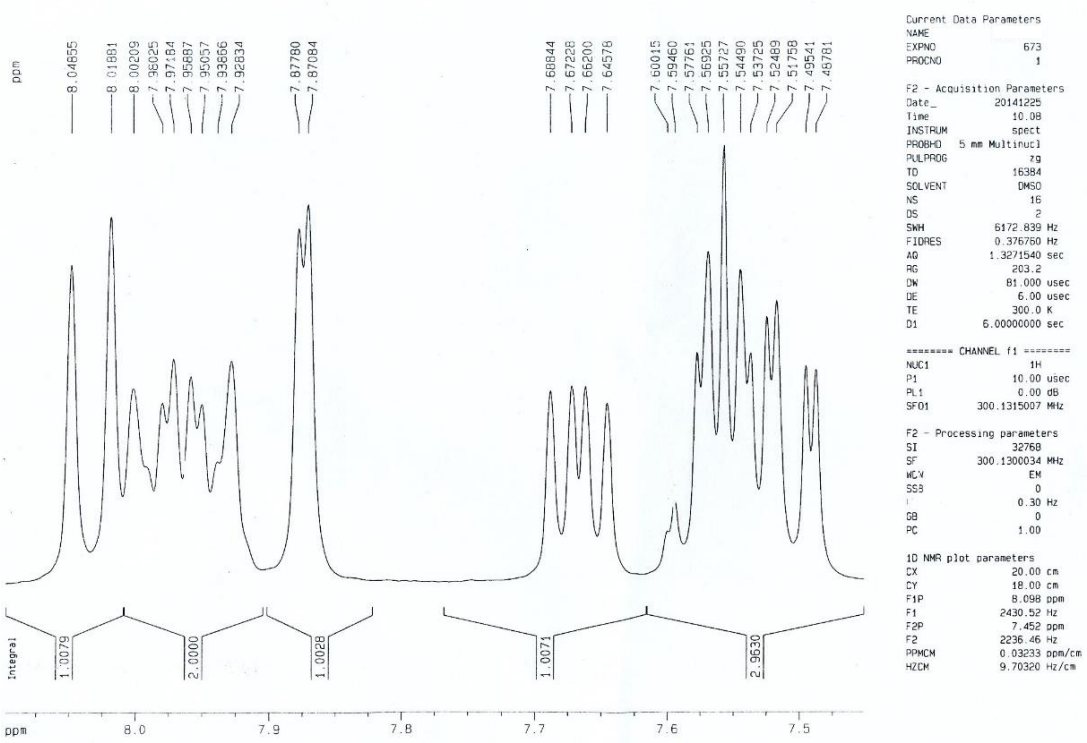
F2 - Processing parameters
SI 32768
SF 300.1300034 MHz
WDW EM
SSB 0
LB 0.30 z
GB 0
PC 1.00

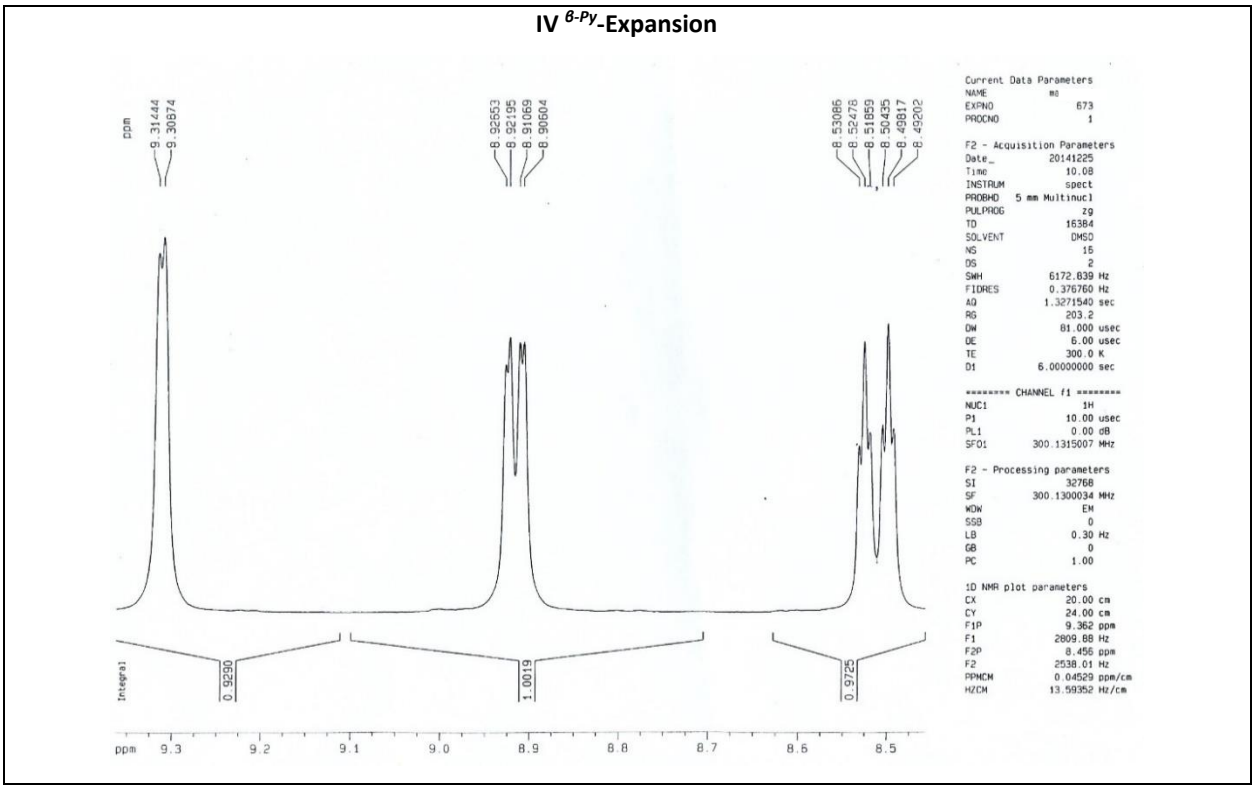
1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 9.480 ppm
F1 2845.32 Hz
F2P 8.511 ppm
F2 2554.52 Hz
PPMCM 0.04845 ppm/cm
HZCM 14.53994 Hz/cm

IV *β-Py*



IV *β-Py*-Expansion

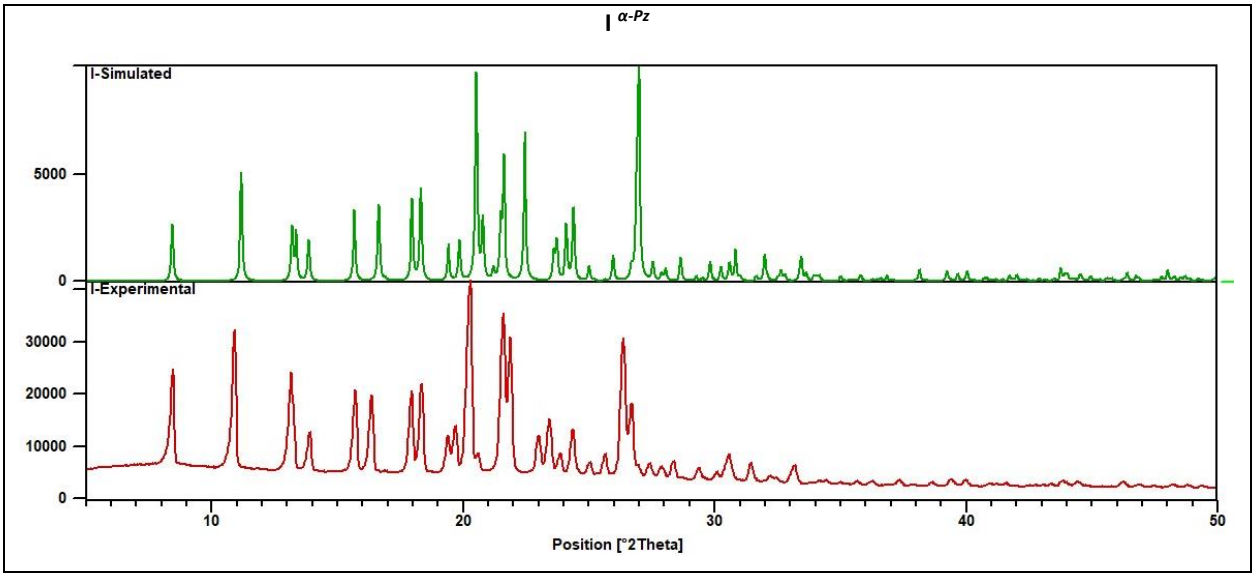


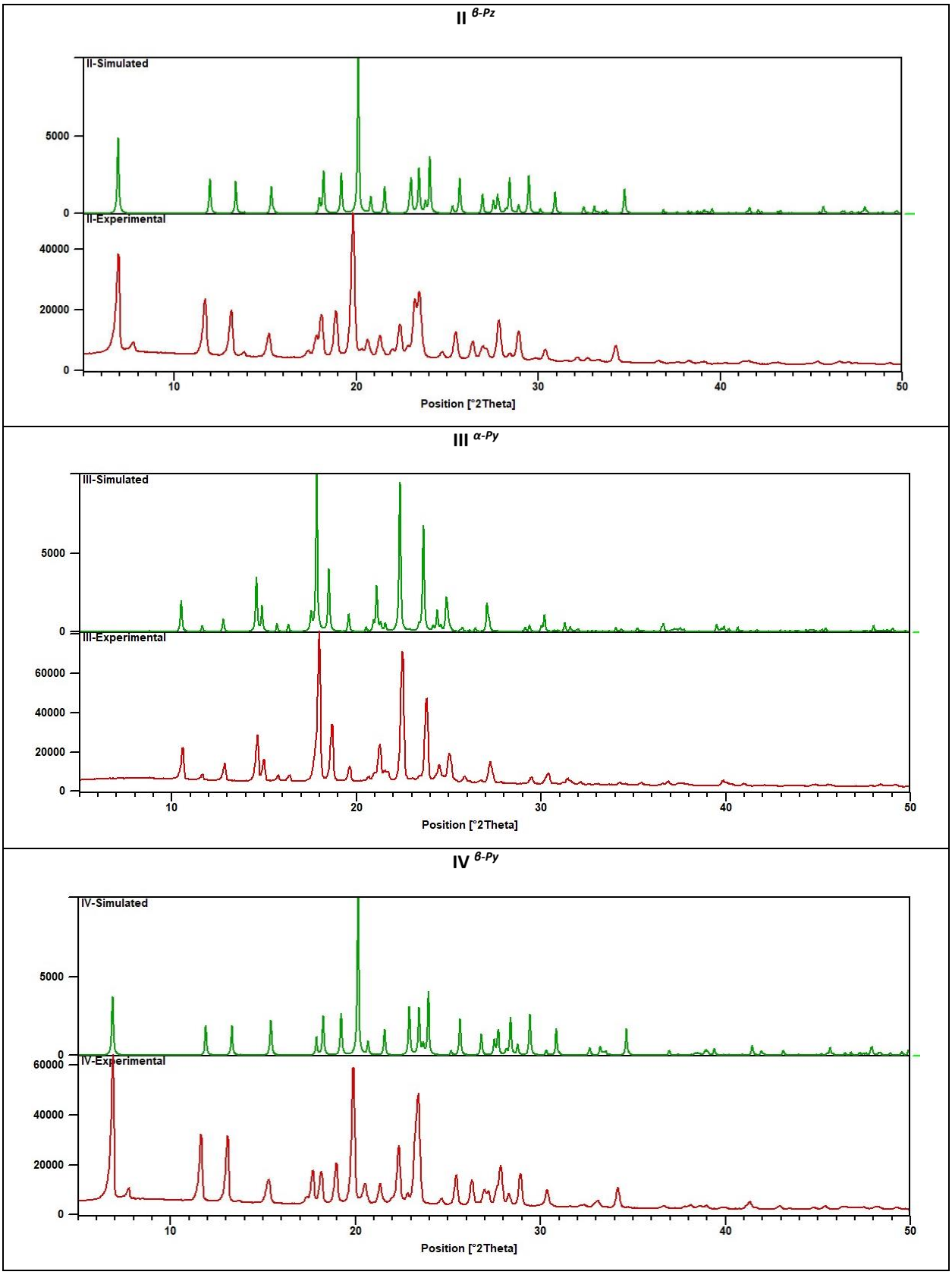


S8. ^{1}H-NMR spectrum interpretation for I $^{\alpha\text{-}Pz}$, II $^{\beta\text{-}Pz}$, III $^{\alpha\text{-}Py}$, IV $^{\beta\text{-}Py}$.

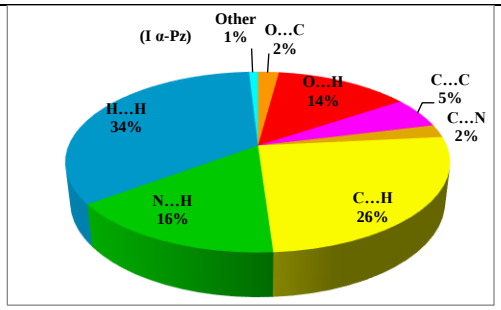
	H_2	H_3	H_3, H_4, H_6	H_7,H_8	H_{15}	H_7	H_8	H_1	H_9	H_6	H_9	H_4	H_{14}	H_{16}	H_{15}	H_{13}
(I $^{\alpha\text{-}Pz}$)	7.54(dd)		7.58(m3H)			7.93(d)	7.99(d)				8.04(dd)		8.97(dd)		9.02(d)	9.50(d)
(II $^{\beta\text{-}Pz}$)		7.54(dd)		7.58(m2H)				7.91(d)	7.97(dd)	8.01(dd)		8.07(d)	8.95(dd)		9.01(d)	9.45(d)
(III $^{\alpha\text{-}Py}$)	7.51(dd)		7.59(m3H)		7.67(dd)	7.91(d)	7.93(d)				8.02(dd)		8.58(dt)	8.95(dd)		9.41(d)
(IV $^{\beta\text{-}Py}$)		7.50(dd)		7.56(m2H)	7.67(dd)			7.87(d)	7.94(dd)	7.99(dd)		8.03(d)	8.51(dt)	8.91(dd)		9.31(d)

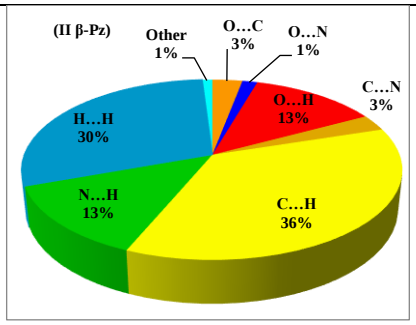
S9. PXRD patterns for I $^{\alpha\text{-}Pz}$, II $^{\beta\text{-}Pz}$, III $^{\alpha\text{-}Py}$, IV $^{\beta\text{-}Py}$.

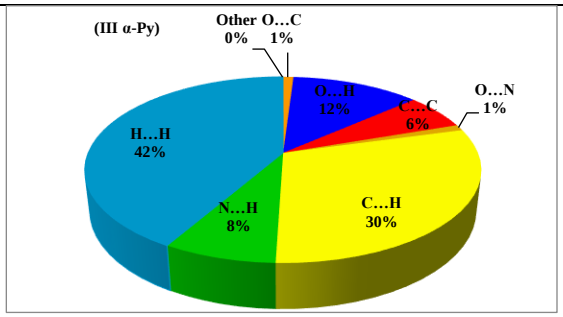


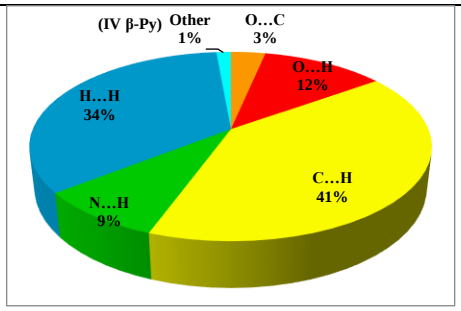

II β-Pz
II-Simulated
II-Experimental
5000
0
40000
20000
0
10
20
30
40
50
Position [°2Theta]
III α-Py
III-Simulated
III-Experimental
5000
0
60000
40000
20000
0
10
20
30
40
50
Position [°2Theta]
IV β-Py
IV-Simulated
IV-Experimental
5000
0
60000
40000
20000
0
10
20
30
40
50
Position [°2Theta]

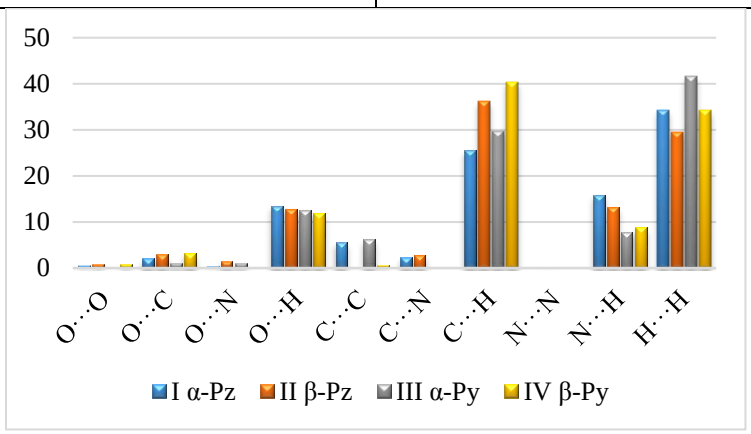
S10. Pi-chart of interactions with Hirschfeld surface analysis for I $^{\alpha\text{-}Pz}$, II $^{\beta\text{-}Pz}$, III $^{\alpha\text{-}Py}$, IV $^{\beta\text{-}Py}$.





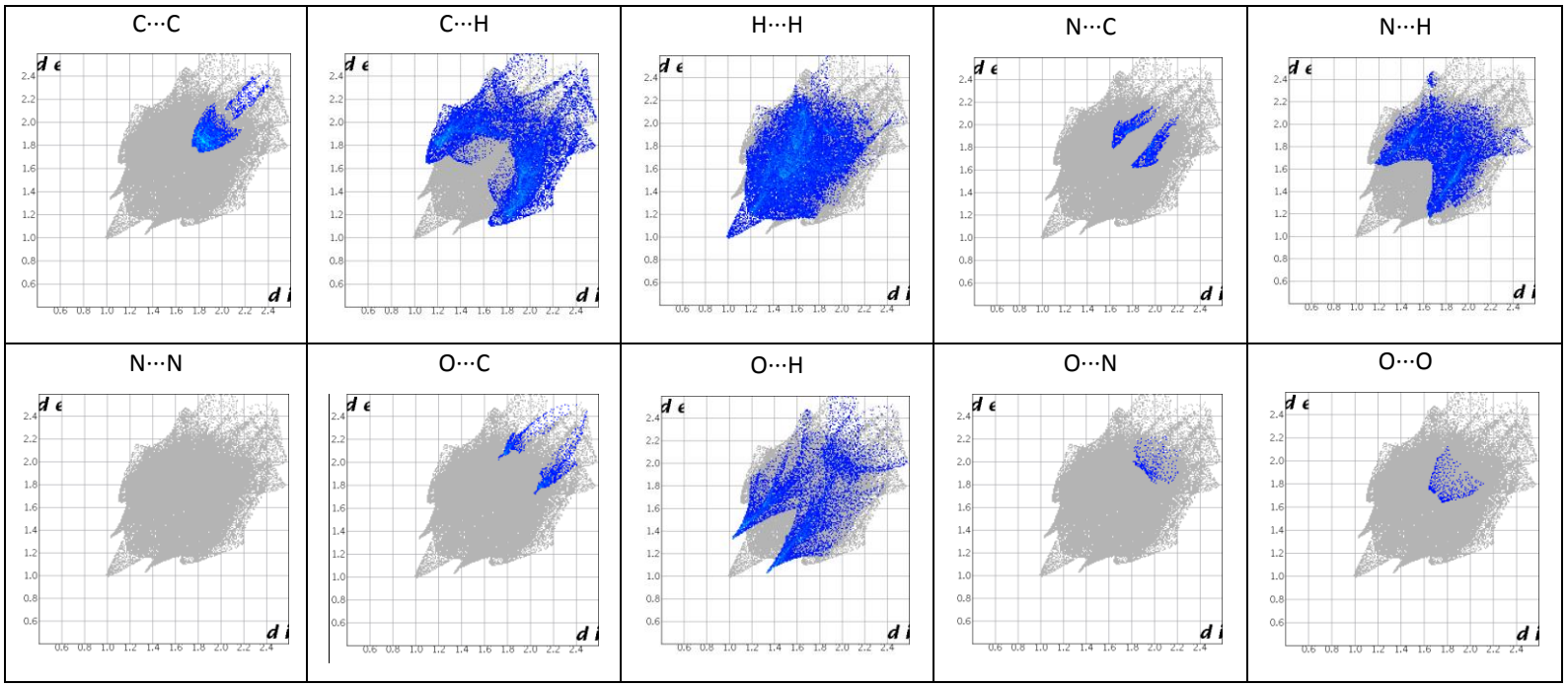




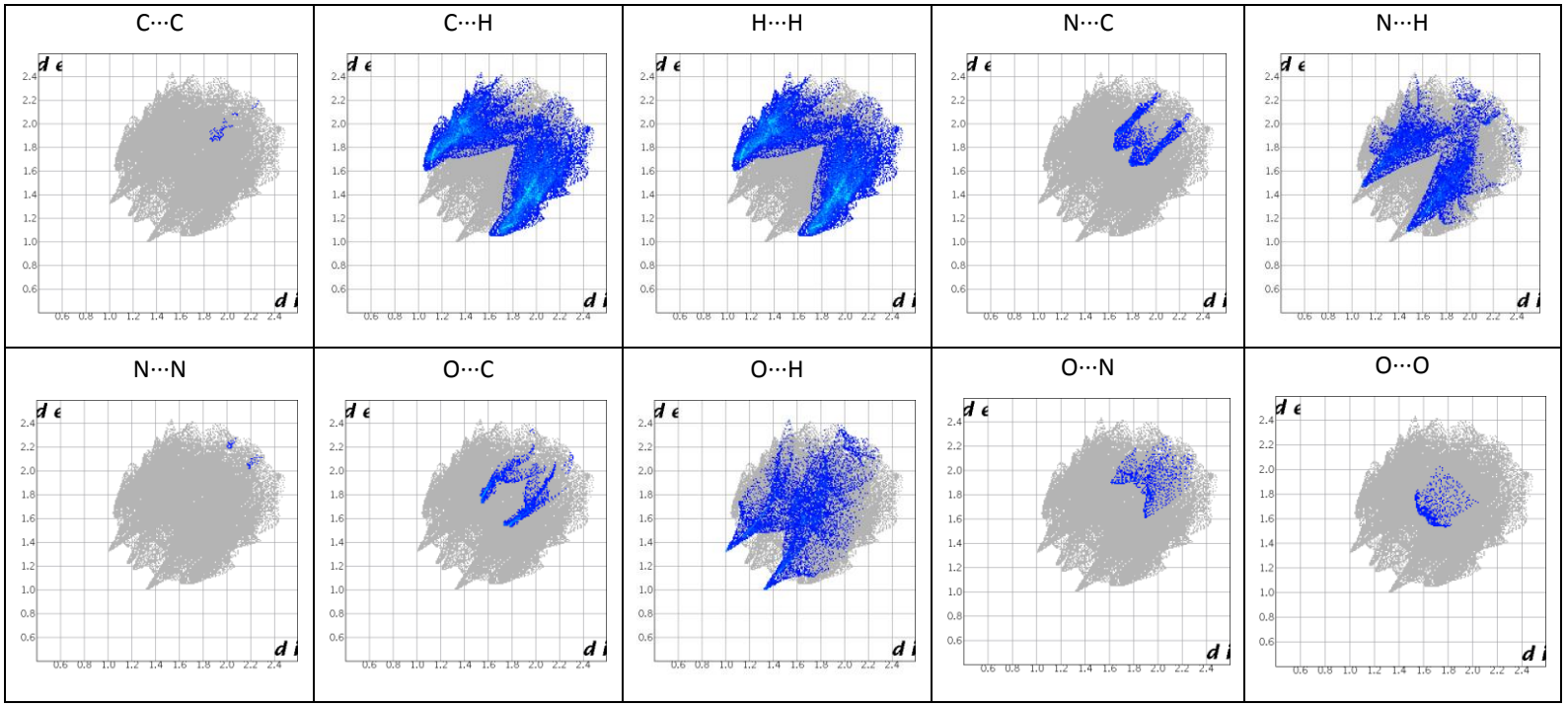


	I $^{\alpha\text{-}Pz}$	II $^{\beta\text{-}Pz}$	III $^{\alpha\text{-}Py}$	IV $^{\beta\text{-}Py}$
O···O	0.5	0.8	0	0.8
O···C	2.1	3	1	3.3
O···N	0.4	1.5	1	0
O···H	13.5	12.7	12.5	11.8
C···C	5.5	0.1	6.2	0.6
C···N	2.3	2.9	0	0
C···H	25.5	36.2	29.7	40.4
N···N	0	0.1	0	0
N···H	15.8	13.2	7.8	8.8

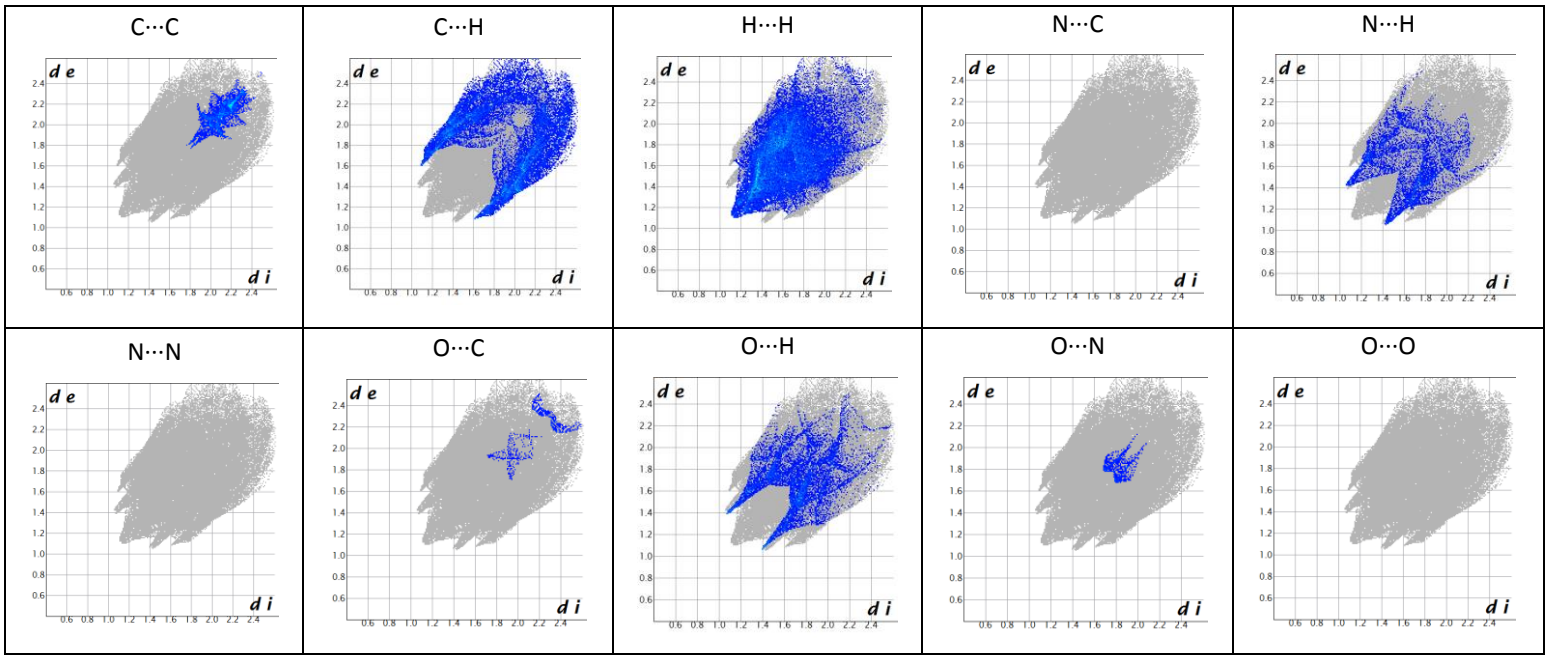
S11. Fingerprint plots of Hirschfeld surface analysis for I $^{\alpha\text{-}Pz}$.



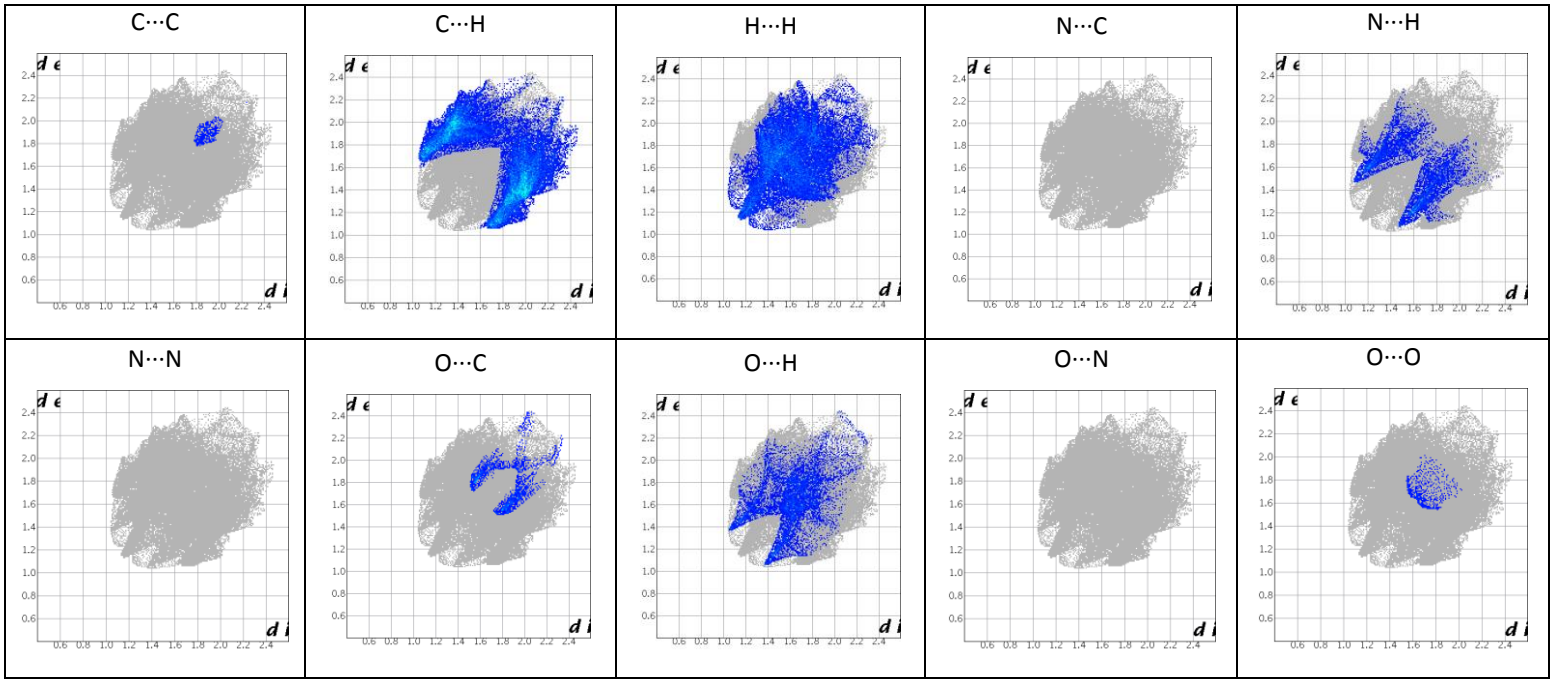
S12. Fingerprint plots of Hirschfeld surface analysis for II $^{\beta\text{-}Pz}$.



S13. Fingerprint plots of Hirschfeld surface analysis for III $^{\alpha\text{-}Py}$.



S14. Fingerprint plots of Hirschfeld surface analysis for IV $^{\beta\text{-}Py}$.



S15. NICS for I $^{\alpha\text{-}Pz}$, II $^{\beta\text{-}Pz}$, III $^{\alpha\text{-}Py}$ and IV $^{\beta\text{-}Py}$.

I $^{\alpha\text{-}Pz}$	II $^{\beta\text{-}Pz}$	III $^{\alpha\text{-}Py}$	IV $^{\beta\text{-}Py}$	Place
-0.4517	-0.4398	-0.4077	-0.4495	Pz or Py (up)
-0.8809	-0.8749	-0.8063	-0.8672	Pz or Py (up)
-1.9551	-1.9593	-1.8145	-1.8975	Pz or Py (up)
-4.9507	-4.9833	-4.7120	-4.7625	Pz or Py (up)
-10.1940	-10.2941	-10.0593	-9.9159	Pz or Py (up)
-5.3489	-5.3935	-6.4528	-6.5976	Pz or Py (mid-centre)
-10.0585	-10.1638	-10.0458	-10.0033	Pz or Py (down)
-4.8303	-5.0057	-4.7221	-4.7565	Pz or Py (down)
-1.8207	-1.9823	-1.7838	-1.8908	Pz or Py (down)
-0.7542	-0.8957	-0.7630	-0.8575	Pz or Py (down)
-0.3444	-0.4623	-0.3639	-0.4367	Pz or Py (down)
-0.6691	-0.6423	-0.6331	-0.6505	Ring 1 (up)
-1.1685	-1.1268	-1.1021	-1.1449	Ring 1 (up)
-2.2883	-2.2346	-2.1462	-2.2762	Ring 1 (up)
-5.1920	-5.1035	-4.8837	-5.1689	Ring 1 (up)
-10.6901	-10.3997	-10.2309	-10.4353	Ring 1 (up)
-9.5743	-9.5055	-9.5076	-9.5673	Ring 1 (mid-centre)
-10.3035	-10.1841	-10.6519	-10.2323	Ring 1(down)
-4.8067	-4.8487	-4.9273	-4.9286	Ring 1(down)
-2.0372	-2.0909	-2.0512	-2.1102	Ring 1(down)
-1.0001	-1.0310	-0.9838	-1.0315	Ring 1(down)
-0.5550	-0.5753	-0.5393	-0.5751	Ring 1(down)
-0.6963	-0.6904	-0.6826	-0.6944	Ring 2 (up)
-1.2112	-1.2149	-1.1870	-1.2114	Ring 2 (up)
-2.3437	-2.3803	-2.3022	-2.3650	Ring 2 (up)
-5.2323	-5.3562	-5.1766	-5.3134	Ring 2 (up)
-10.5022	-10.7019	-10.5233	-10.5215	Ring 2 (up)
-8.4493	-8.4469	-8.4953	-8.4286	Ring 2(mid-centre)
-10.3789	-10.4820	-10.4557	-10.6535	Ring 2 (up)
-5.1904	-5.2906	-5.2281	-5.3618	Ring 2 (up)
-2.3267	-2.3460	-2.3021	-2.3778	Ring 2 (up)
-1.1924	-1.1991	-1.1357	-1.2109	Ring 2 (up)
-0.6753	-0.6873	-0.6165	-0.6887	Ring 2 (up)

S16. HOMA index for I $^{\alpha\text{-}Pz}$, II $^{\beta\text{-}Pz}$, III $^{\alpha\text{-}Py}$, IV $^{\beta\text{-}Py}$.

	HOMA R_1	HOMA R_2	
I $^{\alpha\text{-}Pz}$	0.826	0.785	0.806
II $^{\beta\text{-}Pz}$	0.799	0.834	0.816
III $^{\alpha\text{-}Py}$	0.828	0.784	0.806
IV $^{\beta\text{-}Py}$	0.795	0.819	0.807
β-naphthol	0762	0.712	0.737
α-naphthol	0.759	0.754	0.756

S17. Energy calculations of all the molecular dimers with interaction energy ranking for I $^{\alpha\text{-}Pz}$.

Dimers (I $^{\alpha\text{-}Pz}$)	Ranking	Dimer Energy	Intermolecular Interactions
Dimer4 (D4)	**Rank1**	-8.03	C–H···O C–H···O
Dimer3 (D3)	**Rank2**	-5.75	C–H···π ($R_{2\alpha}$ edge) C–H···O
Dimer1 (D1)	**Rank3**	-5.21	C–H···π ($R_{2\alpha}$ edge) C–H···π (R_{pz} edge)
Dimer5 (D5)	**Rank4**	-2.11	C–H···π ($R_{2\alpha}$ edge)
Dimer2 (D2)	**Rank5**	-0.89	C–H···H

S18. Energy calculations of all the molecular dimers with interaction energy ranking for II $^{\beta\text{-}Pz}$.

Dimers (II $^{\beta\text{-}Pz}$)	Ranking	Dimer Energy	Intermolecular Interactions
Dimer2 (D2)	**Rank1**	-9.16	C–H···π ($R_{1\beta}$ edge) C–H···π (R_{pz} edge) C–H···O
Dimer4 (D4)	**Rank2**	-5.75	C–H···π ($R_{1\beta}$ centre) C–H···π ($R_{2\beta}$ edge) C–H···O
Dimer3 (D3)	**Rank3**	-4.43	C–H···π ($R_{2\beta}$ centre)
Dimer5 (D5)	**Rank4**	-1.78	C–H···π ($R_{2\beta}$ edge) Or C–H···H
Dimer1 (D1)	**Rank5**	-1.40	C–H···N

S19. Energy calculations of all the molecular dimers with interaction energy ranking for III $^{\alpha\text{-}Py}$.

Dimers (III $^{\alpha\text{-}Py}$)	Ranking	Dimer Energy	Intermolecular Interactions
Dimer5 (D5)	Rank1	-6.78	C–H···O
Dimer6 (D6)	Rank2	-6.70	C–H···π ($R_{1\alpha}$ and $R_{2\alpha}$ edge)
Dimer1 (D1)	Rank3	-5.66	C–H···H C–H···N
Dimer3 (D3)	Rank4	-3.11	C–H···π ($R_{1\alpha}$ edge)
Dimer4 (D4)	Rank5	-2.36	C–H···H
Dimer2 (D2)	Rank6	-1.00	C–H···H

S20. Energy calculations of all the molecular dimers with interaction energy ranking for IV $^{\beta\text{-}Py}$.

Dimers (IV $^{\beta\text{-}Py}$)	Ranking	Dimer Energy	Intermolecular Interactions
Dimer2 (D2)	**Rank1**	-8.65	C–H···π ($R_{1\beta}$ edge) C–H···π (R_{pz} centre) C–H···N, C–H···O
Dimer4 (D4)	**Rank2**	-6.90	C–H···π ($R_{2\beta}$ centre) C–H···π ($R_{1\beta}$ edge) C–H···O
Dimer5 (D5)	**Rank3**	-5.44	C–H···H
Dimer3 (D3)	**Rank4**	-4.38	C–H···π ($R_{2\beta}$ centre)
Dimer1 (D1)	**Rank5**	-1.83	C–H···N
Dimer6 (D6)	**Rank6**	-1.77	C–H···H

S21. Energy calculations of 14 molecular tetramers with interaction energy for I $^{\alpha\text{-}Pz}$.

Tetramers (I $^{\alpha\text{-}Pz}$)	Interaction energy	Cooperation Energy
Tetramer1 (D1+D1+D1)	-15.64	-0.30
Tetramer2 (D3+D1+D4)	-19.00	-1.35
Tetramer3 (D3+D3+D3)	-17.25	-0.72
Tetramer4 (D3+D3+D4)	-19.53	-0.68
Tetramer5 (D3D3D5)	-13.61	-1.40
Tetramer6 (D3D5D3)	-13.61	-2.40
Tetramer7 (D4D1D5+D3)	-21.10	-1.36
Tetramer8 (D4D3D4)	-21.81	1.93
Tetramer9 (D4D4D3)	-21.81	-1.09
Tetramer10 (D4D4D5)	-18.17	-2.48
Tetramer11 (D4D5D4)	-18.17	-1.86
Tetramer12 (D5D1D5+D1)	-14.65	-0.47
Tetramer13 (D5D3D5)	-9.97	-1.19
Tetramer14 (D5D4D5)	-12.25	-1.96

S22. Energy calculations of 11 molecular tetramers with interaction energy for II $^{\beta\text{-}Pz}$.

Tetramers (II $^{\beta\text{-}Pz}$)	Interaction energy	Cooperation Energy
Tetramer1 (D1D1D1)	-4.20	-0.06
Tetramer2 (D2D2D2)	-27.48	-1.74
Tetramer3 (D2D2D4)	-24.07	-1.06
Tetramer4 (D2D3D4)	-19.34	-0.06
Tetramer5 (D2D5D2)	-20.11	-0.07
Tetramer6 (D3D3D3)	-13.30	-12.55
Tetramer7 (D4D1D4)	-12.89	0.01
Tetramer8 (D4D2D4)	-20.65	-0.31
Tetramer9 (D4D4D2)	-20.65	-0.13
Tetramer10 (D4D4D4)	-17.24	-0.44
Tetramer11 (D5D5D5)	-5.36	-12.45

S23. Energy calculations of 17 molecular tetramers with interaction energy for III $^{\alpha\text{-}Py}$.

Tetramers (III $^{\alpha\text{-}Py}$)	Interaction energy	Cooperation Energy
Tetramer1 (D1D1D1)	-16.99	-2.85
Tetramer2 (D1D1D3)	-14.43	-1.71
Tetramer3 (D1D1D5)	-18.11	-1.60
Tetramer4 (D1D3D1+D3)	-17.54	-2.77
Tetramer5 (D1D5D1+D4)	-20.48	-0.05
Tetramer6 (D2D2D2)	-3.01	-0.13
Tetramer7 (D3D1D3)	-11.87	-2.82
Tetramer8 (D3D3D1)	-11.87	-2.66
Tetramer9 (D3D3D3)	-9.32	-0.26
Tetramer10 (D3D3D5)	-13.00	-0.07
Tetramer11 (D3D5D3)	-13.00	-0.06
Tetramer12 (D4D4D4)	-7.09	-0.34
Tetramer13 (D5D1D5+D4)	-21.60	-1.18
Tetramer14 (D5D3D5)	-16.68	-0.18
Tetramer15 (D5D5D1)	-19.24	-1.56
Tetramer16 (D5D5D3)	-16.68	-1.32
Tetramer17 (D5D5D5)	-20.36	-2.67

S24. Energy calculations of 17 molecular tetramers with interaction energy for IV $^{\beta\text{-}Py}$.

Tetarmers (IV $^{\beta\text{-}Py}$)	Interaction energy	Cooperation Energy
Tet1 (D1D1D1)	-5.49	-0.09
Tet2 (D2D2D2)	-25.93	-1.55
Tet3 (D2D2D4)	-24.19	-1.35
Tet4 (D2D3D2)	-21.67	-0.25
Tet5 (D2D4D2)	-24.19	-1.15
Tet6 (D3D3D3+2D5)	-24.02	-0.04
Tet7 (D3D5D3)	-14.20	-0.01
Tet8 (D4D3D2+D1)	-17.37	-4.14
Tet9 (D4D3D4)	-18.17	0.05
Tet10 (D4D4D4)	-20.69	-0.70
Tet11 (D4D5D2)	-20.98	-3.90
Tet12 (D4D5D4)	-19.23	-0.63
Tet13 (D5D2D5+D4)	-26.42	-2.71
Tet14 (D5D3D5+2D3)	-24.01	-0.04
Tet15 (D5D5D3+D3)	-19.64	-0.17
Tet16 (D5D5D5)	-16.33	-0.27
Tet17 (D6D6D6+2D5)	-16.21	0.18

S25. Neutron normalized O···H, N···H, C–H···π_e/π_c interaction geometrical parameters for I $^{\alpha\text{-}Pz}$, II $^{\beta\text{-}Pz}$, III $^{\alpha\text{-}Py}$, IV $^{\beta\text{-}Py}$.

Interaction	**D–H/Å**	**H···A/Å**	**D···A/Å**	**∠D–H···A/°**
I $^{\alpha\text{-}Pz}$				
$C_2–H_2\cdots N_2$	1.089	2.973	3.574	115.14
$C_3–H_3\cdots O_{2A}$	1.089	2.909	3.752	134.36
$C_4–H_4\cdots C_8–C_9$ (C_g8)	1.089	2.825	3.556	124.45
$C_9–H_9\cdots C_3–C_4$ (C_g3)	1.089	2.889	3.559	119.92
$C_4–H_4\cdots C_3–C_4$ (C_g3)	1.089	3.004	4.005	152.91
$C_4–H_4\cdots C_4–C_5$ (C_g4)	1.089	3.301	4.235	144.54
$C_{15}–H_{15}\cdots O_1$	1.089	2.495	3.485	150.64
$C_{15}–H_{15}\cdots C_1–C_2$ (C_g1)	1.089	2.919	3.862	145.00
$C_{15}–H_{15}\cdots R_1$	1.089	2.920	3.611	121.57
$C_{14}–H_{14}\cdots C_5–C_6$ (C_g5)	1.089	2.750	3.605	135.15
$C_{14}–H_{14}\cdots C_5–C_{10}$ (C_g11)	1.089	2.808	3.607	130.05
$C_{14}–H_{14}\cdots C_4–C_5$ (C_g4)	1.089	2.981	3.554	113.23
$C_{14}–H_{14}\cdots R_2$	1.089	2.825	3.839	154.80
$C_2–H_2\cdots O_1$	1.089	2.361	3.280	140.99
$C_{13}–H_{13}\cdots O_{2A}$	1.089	2.573	3.472	139.07
$C_9–H_9\cdots N_2$	1.089	3.138	3.997	136.38
$C_8–H_8\cdots N_1$	1.089	3.076	3.792	123.85
$C_{13}–H_{13}\cdots C_1–C_2$ (C_g1)	1.089	3.102	4.178	169.76
$C_{13}–H_{13}\cdots C_{10}–C_1$ (C_g10)	1.089	3.482	4.540	164.35
$C_7–H_7\cdots C_7–C_8$ (C_g7)	1.089	3.017	3.396	100.90
$C_7–H_7\cdots R_2$	1.089	3.433	4.059	117.92
$C_3–H_3\cdots N_1$	1.089	2.875	3.630	126.48
$C_6–H_6\cdots N_1$	1.089	2.830	3.840	154.31
II $^{\beta\text{-}Pz}$				
$C_8–H_8\cdots N_1$	1.089	2.554	3.429	136.76
$C_1–H_1\cdots N_1$	1.089	2.930	3.751	132.33
$C_1–H_1\cdots N_2$	1.089	3.174	3.944	128.45

$C_9–H_9\cdots N_1$	1.089	2.874	3.717	134.26
$C_1–H_1\cdots C_{14}–C_{15}$ (C_g14)	1.089	2.760	3.802	160.11
$C_3–H_3\cdots O_1$	1.089	2.576	3.460	137.64
$C_{13}–H_{13}\cdots O_{2b}$	1.089	2.703	3.221	108.61
$C_{13}–H_{13}\cdots C_2–C_3$ (C_g2)	1.089	2.680	3.643	147.15
$C_6–H_6\cdots C_6–C_7$ (C_g6)	1.089	2.689	3.722	158.02
$C_6–H_6\cdots R_2$	1.089	2.582	3.404	131.54
$C_6–H_6\cdots C_7–C_8$ (C_g7)	1.089	2.794	3.680	138.36
$C_6–H_6\cdots C_5–C_6$ (C_g5)	1.089	2.747	3.653	140.45
$C_{15}–H_{15}\cdots C_1–C_2$ (C_g1)	1.089	2.850	3.779	143.21
$C_{15}–H_{15}\cdots C_2–C_3$ (C_g2)	1.089	2.832	3.731	139.86
$C_{15}–H_{15}\cdots R_1$	1.089	2.821	3.522	122.04
$C_{15}–H_{15}\cdots O_1$	1.089	2.320	3.279	145.77
$C_{14}–H_{14}\cdots C_5–C_9$ (C_g11)	1.089	2.685	3.403	123.01
$C_{14}–H_{14}\cdots C_9–C_{10}$ (C_g9)	1.089	2.619	3.595	148.69
$C_{14}–H_{14}\cdots R_2$	1.089	2.630	3.505	136.91
$C_9–H_9\cdots C_7–C_8$ (C_g7)	1.089	3.142	3.852	123.55
$C_7–H_7\cdots C_8–C_9$ (C_g8)	1.089	3.414	3.824	103.88
$C_8–H_8\cdots C_6–C_7$ (C_g6)	1.089	3.389	4.190	131.48
$C_8–H_8\cdots C_7–C_8$ (C_g7)	1.089	3.201	3.879	121.23
$C_9–H_9\cdots C_8–C_9$ (C_g8)	1.089	3.575	4.411	134.83
$C_8–H_8\cdots R_2$	1.089	3.745	4.623	138.99
$C_4–H_4\cdots N_1$	1.089	2.777	3.589	131.17
III ***α-Py***				
$C_8–H_8\cdots N_1$	1.089	2.459	3.202	124.34
$C_2–H_2\cdots N_1$	1.089	2.849	3.679	132.93
$C_2–H_2\cdots O_{2a}$	1.089	3.465	3.615	89.10
$C_8–H_8\cdots C_{14}–C_{15}$ (C_g15)	1.089	3.293	4.096	131.52
$C_8–H_8\cdots N_1$	1.089	3.517	4.414	140.67
$C_{14}–H_{14}\cdots C_1–C_2$ (C_g1)	1.089	2.732	3.692	146.78
$C_{14}–H_{14}\cdots R_1$	1.089	3.254	4.001	126.65
$C_{14}–H_{14}\cdots O_{2a}$	1.089	3.151	4.069	142.44
$C_{15}–H_{15}\cdots C_3–C_4$ (C_g3)	1.089	3.274	4.176	140.85
$C_{15}–H_{15}\cdots R_1$	1.089	3.336	4.034	123.04
$C_4–H_4\cdots O_1$	1.089	2.792	3.840	161.27
$C_6–H_6\cdots O_1$	1.089	3.125	4.084	147.26
$C_{13}–H_{13}\cdots C_4–C_5$ (C_g4)	1.089	3.166	4.176	154.54
$C_{13}–H_{13}\cdots C_3–C_4$ (C_g3)	1.089	3.365	4.192	133.73
$C_{13}–H_{13}\cdots C_5–C_6$ (C_g5)	1.089	3.408	4.492	173.68
$C_3–H_3\cdots O_1$	1.089	2.434	3.460	156.63
$C_3–H_3\cdots C_{10}–C_1$ (C_g10)	1.089	3.255	4.046	130.32
$C_3–H_3\cdots C_9–C_{10}$ (C_g9)	1.089	3.229	3.777	112.18
$C_3–H_3\cdots C_{10}–C_5$ (C_g11)	1.089	3.206	3.722	110.03
$C_3–H_3\cdots R_1$	1.089	3.479	4.195	124.65
$C_3–H_3\cdots R_2$	1.089	3.371	3.605	93.48
$C_2–H_2\cdots C_4–C_5$ (C_g4)	1.089	3.203	3.869	120.36
$C_2–H_2\cdots C_5–C_6$ (C_g5)	1.089	3.143	3.547	102.81
$C_{15}–H_{15}\cdots C_6–C_7$ (C_g6)	1.089	2.985	3.835	135.09
$C_{16}–H_{16}\cdots C_7–C_8$ (C_g7)	1.089	2.841	3.666	132.53
$C_{16}–H_{16}\cdots C_8–C_9$ (C_g8)	1.089	2.764	3.740	149.03

$C_{16}–H_{16}\cdots R_2$	1.089	3.158	3.907	126.64
$C_{15}–H_{15}\cdots C_7–C_8$ (C_g7)	1.089	3.214	3.853	115.67
$C_{15}–H_{15}\cdots R_2$	1.089	3.485	4.077	118.40
IV ***β-Py***				
$C_8–H_8\cdots N_1$	1.089	2.557	3.410	134.47
$C_9–H_9\cdots N_1$	1.089	2.716	3.562	134.14
$C_1–H_1\cdots C_{14}–C_{15}$ (C_g14)	1.089	2.723	3.780	163.45
$C_3–H_3\cdots O_1$	1.089	2.567	3.480	140.82
$C_{13}–H_{13}\cdots C_2–C_3$ (C_g2)	1.089	2.659	3.568	140.54
$C_6–H_6\cdots C_5–C_6$ (C_g5)	1.089	2.716	3.631	141.40
$C_6–H_6\cdots C_6–C_7$ (C_g6)	1.089	2.660	3.701	159.86
$C_6–H_6\cdots C_7–C_8$ (C_g7)	1.089	2.769	3.679	139.89
$C_6–H_6\cdots R_2$	1.089	2.568	3.405	133.06
$C_{14}–H_{14}\cdots C_8–C_9$ (C_g8)	1.089	2.779	3.836	163.60
$C_{14}–H_{14}\cdots C_5–C_{10}$ (C_g11)	1.089	2.775	3.447	119.74
$C_{14}–H_{14}\cdots C_9–C_{10}$ (C_g9)	1.089	2.675	3.600	142.38
$C_{14}–H_{14}\cdots R_2$	1.089	2.600	3.485	137.90
$C_{15}–H_{15}\cdots R_1$	1.089	2.785	3.506	123.51
$C_{15}–H_{15}\cdots C_1–C_2$ (C_g1)	1.089	2.768	3.732	147.49
$C_{15}–H_{15}\cdots O_1$	1.089	2.428	3.306	136.68
$C_9–H_9\cdots C_6–C_7$ (C_g6)	1.089	3.155	3.820	120.15
$C_6–H_6\cdots C_9–C_{10}$ (C_g9)	1.089	3.142	3.815	120.73
$C_6–H_6\cdots C_{10}–C_1$ (C_g10)	1.089	3.220	3.875	119.56
$C_1–H_1\cdots C_5–C_6$ (C_g5)	1.089	3.230	3.883	119.47
$C_1–H_1\cdots C_4–C_5$ (C_g4)	1.089	3.164	3.835	120.64
$C_4–H_4\cdots C_1–C_2$ (C_g1)	1.089	3.228	3.862	118.05
$C_3–H_3\cdots C_{15}–C_{16}$ (C_g15)	1.089	3.461	4.201	126.50
$C_3–H_3\cdots O_{2b}$	1.089	3.774	4.063	97.59
$C_{16}–H_{16}\cdots O_1$	1.089	3.397	3.379	79.80
$C_{15}–H_{15}\cdots O_1$	1.089	3.204	3.264	83.39
$C_{13}–H_{13}\cdots C_{14}–C_{15}$ (C_g14)	1.089	3.336	3.966	118.05
$C_{15}–H_{15}\cdots C_{12}–C_{13}$ (C_g12)	1.089	3.367	3.367	114.56
$C_8–H_8\cdots C_6–C_7$ (C_g6)	1.089	3.399	4.208	132.16
$C_8–H_8\cdots C_7–C_8$ (C_g7)	1.089	3.182	3.873	122.16
$C_7–H_7\cdots C_8–C_9$ (C_g8)	1.089	3.411	3.830	104.42
$C_8–H_8\cdots C_8–C_9$ (C_g8)	1.089	3.562	3.904	100.16

Natural Bond Orbital Analysis (NBO) has investigated for all of the dimers and has compared with the monomers in all compounds. NBO analysis has shown the charge variations for every interacted atom in the dimers.

S26. NBO analysis for I $^{\alpha\text{-}Pz}$

I $^{\alpha\text{-}Pz}$	Monomer	Dimer1		Dimer2		Dimer3		Dimer4		Dimer5	
O_1	-0.564	-0.567	-0.564	-0.570	-0.586	-0.566	-0.565	-0.571	-0.572	-0.564	-0.563
O_{2a}	-0.528	-0.527	-0.528	-0.529	-0.525	-0.528	-0.528	-0.534	-0.524	-0.528	-0.532
N_1	-0.404	-0.404	-0.404	-0.411	-0.379	-0.404	-0.404	-0.404	-0.403	-0.404	-0.400
N_2	-0.376	-0.376	-0.376	-0.378	-0.404	-0.375	-0.376	-0.391	-0.375	-0.376	-0.387
C_1	0.321	0.312	0.323	0.323	0.321	0.321	0.321	0.300	0.315	0.323	0.321
C_2	-0.219	-0.211	-0.219	-0.221	-0.221	-0.221	-0.211	-0.582	-0.222	-0.219	-0.220
C_3	-0.200	-0.195	-0.196	-0.200	-0.192	-0.191	-0.191	0.647	-0.190	-0.196	-0.191
C_4	-0.164	-0.192	-0.177	-0.166	-0.179	-0.181	-0.181	-0.537	-0.178	-0.177	-0.179
C_5	-0.053	-0.036	-0.034	-0.053	-0.046	-0.046	-0.046	-0.062	-0.059	-0.034	-0.046
C_6	-0.176	-0.182	-0.181	-0.177	-0.174	-0.180	-0.180	-0.175	-0.176	-0.181	-0.175
C_7	-0.200	-0.200	-0.198	-0.200	-0.197	-0.198	-0.198	-0.203	-0.197	-0.198	-0.199
C_8	-0.196	-0.197	-0.196	-0.197	-0.200	-0.204	-0.204	-0.202	-0.194	-0.196	-0.205
C_9	-0.175	-0.179	-0.174	-0.174	-0.173	-0.164	-0.164	-0.164	-0.177	-0.174	-0.172
C_{10}	-0.090	-0.084	-0.096	-0.090	-0.094	-0.096	-0.096	-0.097	-0.103	-0.096	-0.096
C_{11}	0.776	0.774	0.776	0.777	0.786	0.776	0.776	0.786	0.781	0.776	0.778
C_{12}	0.057	0.055	0.057	0.051	0.052	0.057	0.057	0.061	0.055	0.057	0.058
C_{13}	0.057	0.056	0.057	0.051	0.077	0.057	0.057	0.065	0.058	0.057	0.062
C_{14}	0.027	0.027	0.027	0.027	0.027	0.027	0.027	0.025	0.029	0.027	0.037
C_{15}	0.013	0.013	0.013	0.014	0.006	0.013	0.013	0.010	0.014	0.013	0.012
H_2	0.222	0.217	0.223	0.222	0.223	0.223	0.222	0.246	0.226	0.223	0.223
H_3	0.211	0.226	0.209	0.210	0.211	0.211	0.211	0.094	0.215	0.209	0.211
H_4	0.206	0.213	0.204	0.206	0.208	0.207	0.207	0.201	0.212	0.204	0.208
H_6	0.207	0.207	0.204	0.207	0.208	0.207	0.207	0.207	0.212	0.204	0.208
H_7	0.200	0.200	0.198	0.207	0.209	0.217	0.217	0.207	0.212	0.198	0.199
H_8	0.209	0.208	0.209	0.208	0.210	0.210	0.210	0.208	0.212	0.209	0.210
H_9	0.216	0.215	0.216	0.217	0.210	0.214	0.214	0.213	0.218	0.216	0.221
H_{13}	0.220	0.221	0.220	0.216	0.228	0.220	0.220	0.222	0.221	0.220	0.220
H_{14}	0.197	0.197	0.197	0.202	0.194	0.197	0.197	0.197	0.198	0.197	0.196
H_{15}	0.199	0.199	0.199	0.221	0.196	0.199	0.199	0.199	0.199	0.199	0.195

S27. NBO analysis for II $^{\beta\text{-}Pz}$

II $^{\beta\text{-}Pz}$	Monomer	Dimer1		Dimer2		Dimer3		Dimer4		Dimer5	
O_1	-0.569	-0.569	-0.568	-0.523	-0.562	-0.568	-0.568	-0.575	-0.573	-0.569	-0.569
O_{2b}	-0.524	-0.524	-0.523	-0.590	-0.549	-0.523	-0.524	-0.524	-0.522	-0.523	-0.524
N_1	-0.408	-0.409	-0.418	-0.407	-0.412	-0.408	-0.408	-0.415	-0.406	-0.408	-0.408
N_2	-0.375	-0.375	-0.372	-0.378	-0.389	-0.375	-0.375	-0.374	-0.375	-0.375	-0.375
C_1	-0.206	-0.207	-0.206	-0.216	-0.269	-0.200	-0.206	-0.206	-0.212	-0.205	-0.211
C_2	0.295	0.293	0.295	0.296	0.258	0.296	0.294	0.298	0.291	0.296	0.296
C_3	-0.223	-0.225	-0.223	-0.223	-0.238	-0.221	-0.231	-0.222	-0.225	-0.222	-0.224
C_4	-0.159	-0.160	-0.159	-0.157	-0.159	-0.162	-0.149	-0.161	-0.156	-0.160	-0.158
C_5	-0.066	-0.067	-0.066	-0.070	-0.074	-0.074	-0.061	-0.066	-0.075	-0.065	-0.072
C_6	-0.173	-0.173	-0.173	-0.173	-0.173	-0.177	-0.178	-0.173	-0.168	-0.172	-0.172
C_7	-0.206	-0.202	-0.205	-0.204	-0.207	-0.213	-0.204	-0.207	-0.199	-0.210	-0.212
C_8	-0.199	-0.201	-0.198	-0.196	-0.200	-0.202	-0.196	-0.200	-0.194	-0.203	-0.183
C_9	-0.178	-0.169	-0.178	-0.185	-0.186	-0.169	-0.182	-0.178	-0.187	-0.177	-0.194
C_{10}	-0.048	-0.055	-0.048	-0.038	-0.072	-0.053	-0.053	-0.048	-0.064	-0.049	-0.034
C_{11}	0.775	0.774	0.775	0.785	0.783	0.775	0.775	0.776	0.779	0.775	0.775
C_{12}	0.056	0.057	0.059	0.056	0.060	0.056	0.057	0.049	0.054	0.056	0.056
C_{13}	0.060	0.060	0.064	0.076	0.066	0.061	0.060	0.054	0.062	0.061	0.060
C_{14}	0.030	0.030	0.031	0.033	0.021	0.031	0.030	0.030	0.032	0.031	0.030
C_{15}	0.013	0.013	0.015	0.010	0.013	0.014	0.013	0.010	0.014	0.013	0.013
H_1	0.222	0.221	0.222	0.217	0.207	0.224	0.221	0.222	0.223	0.222	0.221
H_3	0.223	0.222	0.223	0.223	0.244	0.224	0.221	0.223	0.227	0.224	0.223
H_4	0.210	0.209	0.210	0.209	0.208	0.210	0.208	0.209	0.214	0.210	0.210
H_6	0.207	0.205	0.207	0.206	0.206	0.210	0.215	0.206	0.211	0.208	0.207
H_7	0.208	0.206	0.208	0.208	0.207	0.210	0.210	0.207	0.212	0.213	0.209
H_8	0.209	0.220	0.209	0.209	0.208	0.211	0.208	0.208	0.212	0.205	0.215
H_9	0.207	0.203	0.208	0.214	0.205	0.211	0.206	0.207	0.211	0.208	0.202
H_{13}	0.222	0.222	0.221	0.220	0.225	0.222	0.222	0.217	0.224	0.222	0.222
H_{14}	0.198	0.197	0.197	0.195	0.199	0.198	0.197	0.203	0.198	0.198	0.198
H_{15}	0.198	0.198	0.199	0.195	0.201	0.198	0.198	0.222	0.199	0.198	0.198

S28. NBO analysis for III $^{\alpha\text{-}Py}$

III $^{\alpha\text{-}Py}$	Monomer	Dimer1		Dimer2		Dimer3		Dimer4		Dimer5	
O_1	-0.570	-0.567	-0.566	-0.571	-0.569	-0.872	-0.573	-0.569	-0.579	-0.690	-0.584
O_{2a}	-0.558	-0.556	-0.566	-0.558	-0.558	-0.598	-0.559	-0.558	-0.556	-0.741	-0.553
N_1	-0.437	-0.451	-0.450	-0.437	-0.437	-0.436	-0.546	-0.438	-0.430	-0.438	-0.436
C_1	0.321	0.287	0.319	0.323	0.321	0.285	0.322	0.317	0.320	0.744	0.318
C_2	-0.224	-0.655	-0.226	-0.223	-0.223	-0.245	-0.224	-0.231	-0.224	-0.487	-0.227
C_3	-0.193	-0.192	-0.197	-0.193	-0.193	-0.196	-0.193	-0.180	-0.192	-0.224	-0.194
C_4	-0.176	-0.420	-0.175	-0.177	-0.176	-0.183	-0.177	-0.187	-0.175	-0.289	-0.186
C_5	-0.047	-0.085	-0.049	-0.047	-0.047	-0.048	-0.047	-0.050	-0.047	-1.733	-0.047
C_6	-0.174	-0.174	-0.176	-0.174	-0.174	-0.179	-0.174	-0.173	-0.174	-0.119	-0.179
C_7	-0.197	-0.202	-0.195	-0.198	-0.197	-0.195	-0.198	-0.207	-0.197	-0.121	-0.189
C_8	-0.199	-0.195	-0.195	-0.199	-0.199	-0.191	-0.200	-0.176	-0.199	-0.191	-0.185
C_9	-0.164	-0.177	-0.175	-0.162	-0.165	-0.176	-0.164	-0.192	-0.165	0.778	-0.184
C_{10}	-0.092	-0.099	-0.090	-0.091	-0.092	-0.095	-0.092	-0.078	-0.092	-0.307	-0.098
C_{11}	0.799	0.795	0.799	0.799	0.799	1.519	0.798	0.798	0.802	0.263	0.805
C_{12}	-0.189	-0.191	-0.189	-0.189	-0.187	-0.558	-0.197	-0.188	-0.191	-0.292	-0.190
C_{13}	0.094	0.103	0.087	0.093	0.095	0.088	0.072	0.093	0.092	0.090	0.093
C_{14}	0.066	0.060	0.065	0.066	0.063	0.068	-0.219	0.065	0.069	0.066	0.067
C_{15}	-0.234	-0.234	-0.233	-0.233	-0.233	-0.233	-0.335	-0.234	-0.233	-0.235	-0.233
C_{16}	-0.154	-0.152	-0.151	-0.153	-0.153	-0.176	-0.154	-0.154	-0.154	-0.160	-0.152
H_2	0.223	0.223	0.221	0.223	0.223	0.226	0.223	0.221	0.223	0.066	0.222
H_3	0.211	-0.103	0.210	0.211	0.211	0.213	0.211	0.212	0.212	0.238	0.211
H_4	0.208	0.196	0.207	0.208	0.208	0.209	0.208	0.215	0.209	0.207	0.207
H_6	0.208	0.207	0.206	0.207	0.208	0.208	0.208	0.218	0.208	0.123	0.206
H_7	0.209	0.207	0.207	0.205	0.209	0.209	0.208	0.207	0.209	0.205	0.219
H_8	0.209	0.208	0.233	0.207	0.210	0.211	0.209	0.206	0.210	0.187	0.210
H_9	0.209	0.209	0.207	0.211	0.209	0.214	0.209	0.208	0.209	0.097	0.208
H_{13}	0.216	0.220	0.212	0.216	0.216	0.215	0.211	0.216	0.212	0.212	0.215
H_{14}	0.191	0.190	0.192	0.191	0.189	0.191	0.176	0.191	0.193	0.191	0.192
H_{15}	0.209	0.209	0.210	0.210	0.209	0.212	0.197	0.209	0.210	0.210	0.210
H_{16}	0.235	0.238	0.237	0.235	0.236	0.241	0.232	0.235	0.235	0.240	0.236

S29. NBO analysis for IV $^{\beta\text{-}Py}$

IV $^{\beta\text{-}Py}$	Monomer	Dimer1		Dimer2		Dimer3		Dimer4		Dimer5		Dimer6	
O_1	-0.568	-0.567	-0.568	0.296	-0.598	-0.568	-0.568	-0.583	-0.574	-0.569	-0.571	-0.568	-0.568
O_{2b}	-0.559	-0.559	-0.559	-0.654	-0.567	-0.560	-0.558	-0.554	-0.558	-0.558	-0.564	-0.559	-0.559
N_1	-0.448	-0.459	-0.449	-0.458	-0.445	-0.449	-0.448	-0.447	-0.456	-0.447	-0.449	-0.448	-0.448
C_1	-0.206	-0.206	-0.207	-0.202	-0.255	-0.762	-0.195	-0.213	-0.206	-0.198	0.619	-0.211	-0.206
C_2	0.297	0.296	0.294	0.291	0.274	0.294	0.296	0.291	0.300	0.293	-0.144	0.297	0.298
C_3	-0.223	-0.224	-0.227	-0.247	-0.228	-0.226	-0.222	-0.226	-0.222	-0.223	-0.235	-0.224	-0.222
C_4	-0.158	-0.158	-0.158	-0.157	-0.159	-0.161	-0.161	-0.152	-0.160	-0.159	-0.158	-0.158	-0.158
C_5	-0.066	-0.066	-0.067	-0.068	-0.072	-0.057	-0.081	-0.072	-0.067	-0.072	-0.081	-0.072	-0.066
C_6	-0.172	-0.172	-0.175	-0.172	-0.176	-0.175	-0.177	-0.166	-0.172	-0.177	-0.171	-0.171	-0.172
C_7	-0.206	-0.205	-0.198	-0.207	-0.204	-0.205	-0.213	-0.199	-0.207	-0.207	-0.206	-0.211	-0.210
C_8	-0.199	-0.198	-0.200	-0.202	-0.197	-0.196	-0.202	-0.194	-0.200	-0.198	-0.200	-0.183	-0.203
C_9	-0.178	-0.178	-0.170	-0.180	-0.184	-0.179	-0.173	-0.186	-0.178	-0.178	-0.199	-0.194	-0.176
C_{10}	-0.047	-0.047	-0.054	-0.058	-0.065	-0.057	-0.044	-0.060	-0.047	-0.051	-0.177	-0.033	-0.048
C_{11}	0.794	0.794	0.794	0.121	0.795	0.796	0.795	0.801	0.795	0.792	0.797	0.794	0.794
C_{12}	-0.200	-0.198	-0.199	-0.244	-0.210	-0.200	-0.200	-0.203	-0.206	-0.203	-0.200	-0.200	0.200
C_{13}	0.106	-0.127	0.105	0.093	0.108	0.106	0.106	0.107	0.100	0.102	0.107	0.105	0.106
C_{14}	0.074	-0.245	0.073	0.060	0.076	0.074	0.075	0.077	0.071	0.075	0.074	0.074	0.074
C_{15}	-0.248	0.075	-0.249	-0.253	-0.251	-0.248	-0.248	-0.247	-0.249	-0.247	-0.242	-0.248	-0.248
C_{16}	-0.129	0.110	-0.129	-0.147	-0.131	-0.129	-0.129	-0.128	-0.125	-0.129	-0.117	-0.129	0.219
H_1	0.221	0.221	0.219	0.217	0.208	0.214	0.222	0.223	0.222	0.224	0.011	0.220	0.222
H_3	0.223	0.223	0.221	0.242	0.220	0.221	0.224	0.225	0.223	0.215	0.222	0.223	0.224
H_4	0.210	0.210	0.209	0.208	0.209	0.210	0.212	0.213	0.209	0.216	0.208	0.210	0.211
H_6	0.207	0.207	0.205	0.207	0.206	0.216	0.210	0.211	0.206	0.213	0.207	0.207	0.208
H_7	0.209	0.209	0.212	0.207	0.208	0.210	0.211	0.213	0.208	0.210	0.208	0.209	0.214
H_8	0.208	0.209	0.220	0.207	0.209	0.206	0.210	0.212	0.208	0.209	0.207	0.215	0.204
H_9	0.208	0.208	0.202	0.207	0.218	0.206	0.211	0.211	0.208	0.208	0.211	0.202	0.208
H_{13}	0.213	0.231	0.213	0.215	0.215	0.213	0.213	0.212	0.208	0.215	0.212	0.213	0.213
H_{14}	0.191	0.189	0.190	0.191	0.191	0.191	0.191	0.192	0.194	0.192	0.191	0.191	0.191
H_{15}	0.218	0.219	0.217	0.218	0.218	0.217	0.218	0.219	0.237	0.219	0.211	0.218	0.218
H_{16}	0.230	0.212	0.230	0.231	0.230	0.230	0.229	0.230	0.234	0.230	0.220	0.230	0.230