

SUPPORTING INFORMATION

Halogen-bonding complexes based on bis(iodoethynyl)benzene units: A new versatile route to supramolecular materials.

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Experimental Section

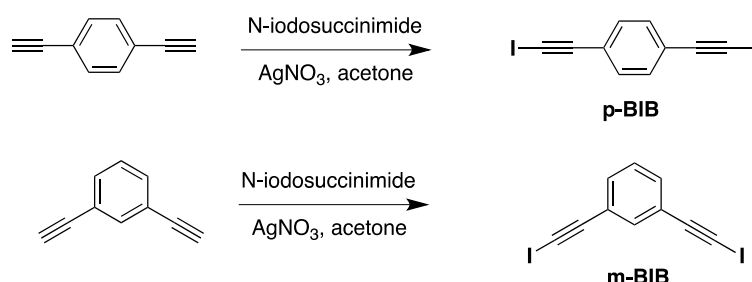
Materials and Methods.

All commercial reagents were used as purchased. FT-IR spectra were recorded on a Bruker Vertex spectrophotometer. ^1H and ^{13}C NMR spectra were recorded on a Bruker Avance 400 spectrometer or a Bruker Avance 300 spectrometer. The mesophase identification was based on microscopic examination of the textures formed by samples between two glass plates. NIKON and OLYMPUS BH-2 polarizing microscopes equipped with a LINKAM THMS600 hot stage were used. The temperatures and enthalpies of the phase transitions were determined by calorimetric measurements performed with DSC TA Instrument Q-20 and Q-2000 systems. Thermogravimetric analysis (TGA) was performed using a TA Q5000IR instrument at a heating rate of 10 $^{\circ}\text{C}$ /min under a nitrogen atmosphere. The X-ray investigations on non-oriented samples were carried out in Lindemann capillary tubes (diameter: 0.9 or 1 mm) using a PINHOLE (ANTON-PAAR) film camera. XPS instrument is a Kratos Aris Ultra DLD. The X-ray source was run at 12 kV and 10 mA. All core-level spectra were referenced to the C 1s neutral carbon peak at a binding energy of 285.0 eV in order to compensate for surface charge effects. The pressure in the analysis chamber was maintained under ultrahigh vacuum below 10^{-9} mbar.

X-ray quality single crystals were obtained by slow evaporation of solutions of complexes P-Py1-10 and P-BN-10 in CH_3CN . The crystals are air stable and were mounted on the tip of a glass fibre using epoxy cement. X-ray diffraction experiments were carried out on an Oxford-diffraction Xcalibur S diffractometer. Data were collected at 150(2) K with Mo- $\text{K}\alpha$ radiation. Software packages XSCANS¹ and CrysAlis² were used to process data.

S1. Synthesis and characterization of the XB-donors and XB-acceptors

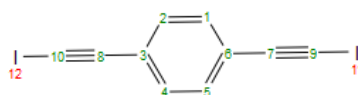
Scheme S1. Synthesis of the XB-donors *p*-BIB and *m*-BIB



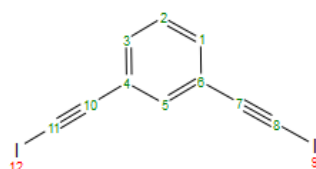
General Procedure for the preparation of bis(iodoethynyl)benzene

N-Iodosuccinimide (4.14 g, 36.2 mmol) and silver nitrate (0.62 g, 3.62 mmol) were added successively to a solution of corresponding diethynylbenzene (2.28 g, 18.1 mmol) in acetone. The reaction mixture was stirred at 0°C for 5 h. The crude was filtered and washed with diethylether, afterwards the solvent was removed under reduce pressure. The residue was extracted with dicloromethane (3 x 50 mL) and water (50 mL). Then, the organic layer was dried over MgSO₄ and evaporated. The pure products were recovered as yellow solids.

1,4-bis(Iodoethynyl)benzene (*p*-BIB) Yield: 75%. Mp (°C): 129. ¹H NMR (300 MHz, CDCl₃) δ 7.36 (s, 4H); ¹³C NMR (75 MHz, CDCl₃) δ 9.1 (9, 10), 93.7 (7, 8), 123.9 (3, 6), 132.3 (1, 2, 4, 5).



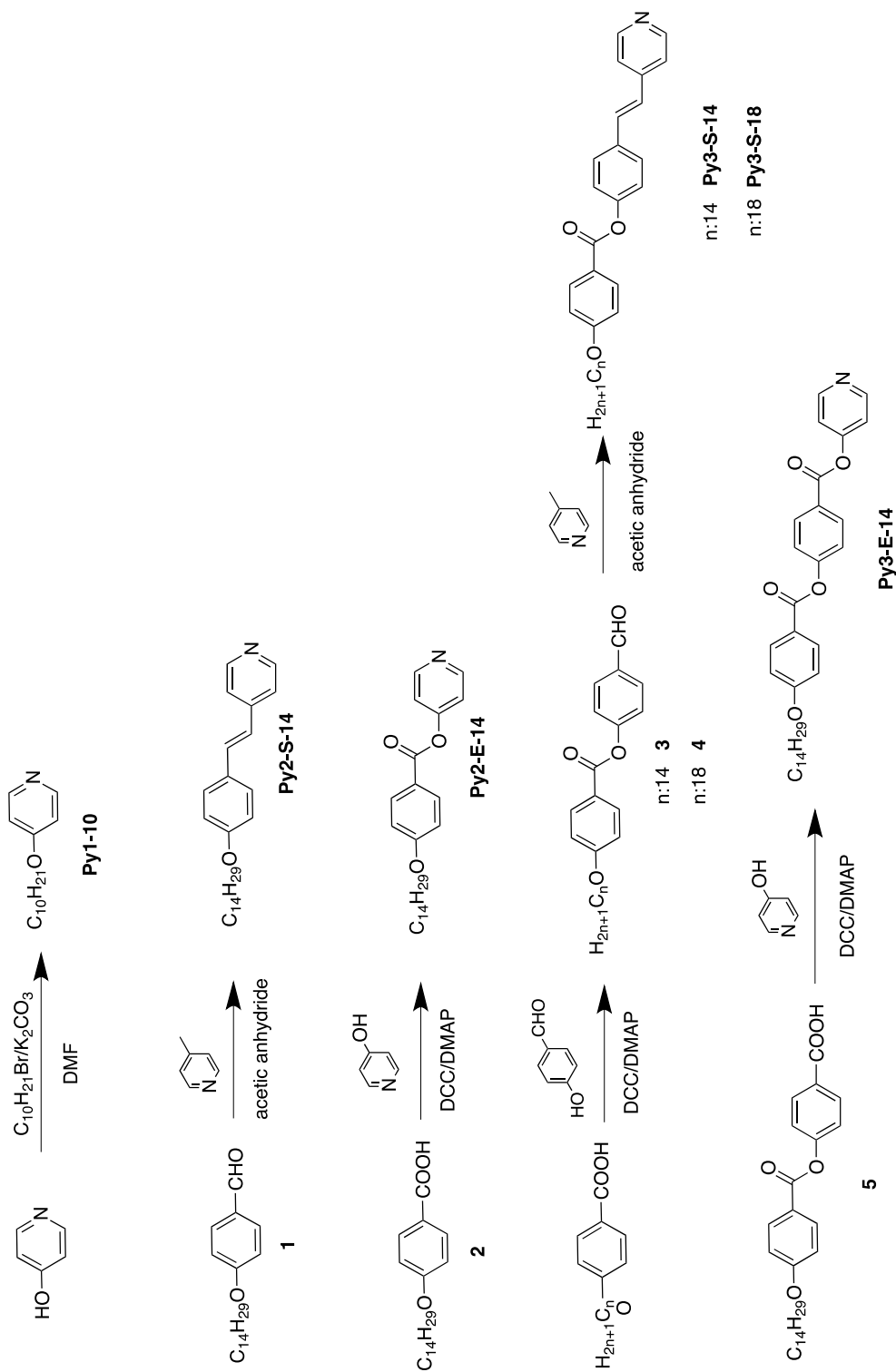
1,3-bis(Iodoethynyl)benzene (*m*-BIB) Yield: 80%. Mp (°C): 88. ¹H NMR (300 MHz, CDCl₃-*d*) δ 7.50 (t, *J* = 1.6 Hz, 1H (5)), 7.40 – 7.35 (m, 2H (1,3)), 7.25 (td, *J* = 6.6, 1.1 Hz, 1H (2)); ¹³C NMR (75 MHz, CDCl₃) δ 7.8 (8, 11), 93.2 (7, 10), 123.8 (4, 6), 128.4 (1, 3), 132.7 (2), 136.2 (5).



Synthetic Procedures for the preparation of XB-acceptors

The synthetical pathways used to prepare the different pyridine derivatives are shown in Scheme S2. Compounds **1-4** have been previously described³⁻⁵ and our data are in agreement with those reported.

Scheme S2. Synthesis of the XB-acceptors.



4-(n-Decyloxy)pyridine (Py1-10). 4-Hydroxypyridine (5.00 g, 52.6 mmol) and of anhydrous potassium carbonate (21.79 g, 157.9 mmol) were stirred in 95 mL of dry DMF. The flask was heated to 100°C under inert atmosphere and then 1-bromodecane (13.97 g, 63.2 mmol) was added slowly. The mixture was stirred at 100°C for six hours. Then it was allowed to cool to room temperature and extracted with a mixture of hexane/ ethyl acetate (1:1). The organic mixture was washed with NaOH (10%), washed with brine, dried over MgSO₄, filtered and the solvent was evaporated. The resulting product was purified by column chromatography using hexane/ dichloromethane (3:2) as eluent to give a red oil. Yield: 3.5g (70%). ¹H NMR (300 MHz, CDCl₃) δ 0.88 (t, *J* = 6.7 Hz, 3H), 1.28-1.43 (m, 14H), 1.79 (m, 2H), 4.00 (t, *J* = 6.5 Hz, 2H), 6.79 (d, *J* = 4.9 Hz, 2H), 8.41 (d, *J* = 4.6 Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 14.0, 22.6, 25.9, 28.8, 29.3, 29.5, 31.8, 67.8, 110.2, 150.9, 165.0. MS (ESI-MS) *m/z*: 236 [M+H]⁺

4-[2-[4-(n-Tetradecyloxy)phenyl]ethenyl]pyridine (Py2-S-14). Compound **1** (1.35 g, 3.1 mmol) and picoline (0.29 g, 3.1 mmol) were refluxed in acetic anhydride for 48 hours. Then the reaction mixture was cooled down to room temperature, the solid filtered and recrystallized from ethyl acetate to yield a yellowish solid. Yield: 3.0 g (30%). Mp (°C): 89. ¹H NMR (400 MHz, CDCl₃) δ 0.88 (t, *J* = 6.0Hz, 3H), 1.27 – 1.45 (m, 22H), 1.80 (m, 2H), 3.98 (t, *J* = 6.0Hz, 2H), 6.86 (d, *J* = 16Hz, 1H), 6.90 (d, *J* = 8Hz, 2H), 7.24 (d, *J* = 16.0 Hz, 1H), 7.32 (d, *J* = 8.0Hz, 2H), 7.46 (d, *J* = 8.0Hz, 2H), 8.53 (d, *J*=8.0Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 14.1, 22.7, 26.0, 29.2, 29.3, 29.4, 29.5, 29.6, 29.7, 29.8, 31.9, 68.1, 114.8, 120.6, 123.5, 128.4, 128.7, 132.9, 145.1, 150.0, 159.8.

4-Pyridinyl-4-(n-tetradecyloxy)benzoate (Py2-E-14). Compound **2** (0.50 g, 1.4 mmol), 4-hydroxypyridine (0.13 g, 1.4 mmol) and DMAP (0.02 g, 0.14 mmol) of were dissolved in 50 mL dry dichloromethane in an ice bath. The reaction mixture was stirred under argon atmosphere for 30 min. Then, DCC (0.32 g, 1.5 mmol) was added and the reaction stirred at room temperature for 24 h. After this time, the solid was filtered off and the solvent evaporated. The crude product was purified by flash chromatography using dichloromethane as eluent to yield a white solid. Yield: 0.25 g (43%). Mp (°C): 75. ¹H NMR (300 MHz, CDCl₃) δ 0.89 (t, *J* = 6.0Hz, 3H), 1.27 – 1.49 (m, 22H), 1.84 (m, 2H), 4.05 (t, *J* = 6.0Hz, 2H), 6.99 (d, *J* = 8.9Hz, 2H), 7.26 (d, *J* = 5.1 Hz, 2H), 8.13 (d, *J* = 9.0Hz, 2H), 8.68 (d, *J* = 5.1Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 14.1, 22.7,

26.0, 29.0, 29.3, 29.5, 29.6, 29.7, 31.9, 68.4, 114.5, 117.2, 120.6, 132.5, 151.3, 158.1, 163.8, 164.0.

4-(2-(Pyridin-4-yl)vinyl)phenyl-4-(n-tetradecyloxy)benzoate (Py3-S-14). Compound **3** (1.35 g, 3.1 mmol) and picoline (0.287 g, 3.1 mmol) were refluxed in acetic anhydride for 48 hours. Then the reaction mixture is cooled down to room temperature, the solid filtered and recrystallized from ethyl acetate to yield a yellowish solid. Yield: 0.70 g (44%). Mp (°C): Cr 108 SmA 172 I. ¹H NMR (300 MHz, CDCl₃) δ 0.90 (t, *J* = 6.0Hz, 3H), 1.27 – 1.60 (m, 30H), 1.83 (m, 2H), 4.07 (t, *J* = 6.0Hz, 2H), 6.99-7.05 (m, 3H), 7.23 (m, 2H), 7.41(m, 3H), 7.62 (d, *J* = 9.0Hz, 2H), 8.18 (d, *J* = 9.0Hz, 2H), 8.54 (d, *J* = 6.0Hz, 2H). MS (FAB-MS) *m/z*: 514 [M+H]⁺

4-(2-(Pyridin-4-yl)vinyl)phenyl 4-(n-octadecyloxy)benzoate (Py3-S-18). Compound **4** (1.00 g, 2.0 mmol) and picoline (0.23 g, 2.4 mmol) of were refluxed in acetic anhydride for 48 hours. Then the reaction mixture is cooled down to room temperature, the solid filtered and recrystallized from ethyl acetate to yield a yellowish solid. Yield: 0.50 g (43%). Mp (°C): Cr 109 SmA 168 I. ¹H NMR (300 MHz, CDCl₃) δ 0.90 (t, *J* = 6.0Hz, 3H) 1.27 – 1.60 (m, 30H), 1.83 (m, 2H), 4.07 (t, *J* = 6.0Hz, 2H), 6.99-7.05 (m, 3H), 7.23 (m, 2H), 7.41(m, 3H), 7.62 (d, *J* = 9.0Hz, 2H), 8.18 (d, *J* = 9.0Hz, 2H), 8.54 (d, *J* = 6.0Hz, 2H). MS (FAB-MS) *m/z*: 570 [M+H]⁺

4-Pyridinyl-4-[(4-(n-tetradecyloxy)benzoyl)oxy]benzoate (Py3-E-14). Compound **5** (0.50 g, 1.1 mmol), 4-hydroxypyridine (0.10 g, 1.1 mmol) and DMAP (0.01 g, 0.11 mmol) were dissolved in 50 mL dry dichloromethane in an ice bath. The reaction mixture was stirred under argon atmosphere for 30 min. Then, DCC (0.27 g, 1.3 mmol) was added and the reaction stirred at rom temperature for 24 h. After this time, the solid was filtered off and the solvent evaporated. The crude product was purified by flash chromatography using dichloromethane as eluent to yield a white solid. Yield: 0.25 g (43%). Mp (°C): Cr 124 SmA 139 I. ¹H NMR (400 MHz, CDCl₃) δ 0.90 (t, *J* = 6.0Hz, 3H) 1.27 – 1.60 (m, 22H), 1.83 (m, 2H), 4.07 (t, *J* = 8.0Hz, 2H), 7.00 (d, *J* = 8.0Hz, 2H), 7.23 (d, *J* = 4.0Hz, 2H), 7.41(d, *J* = 8.0Hz, 2H), 8.16 (d, *J* = 8.0Hz, 2H), 8.28 (d, *J* = 8.0Hz, 2H), 8.70 (d, *J* = 4.0Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 14.1, 22.7, 26.0, 29.1, 29.3, 29.4, 29.5, 2.6, 29.7, 29.8, 31.9, 68.4, 114.4, 117.1, 120.8, 122.3, 126.0, 132.0, 132.5, 151.5, 155.8, 157.8, 163.1, 163.9, 164.2. MS (FAB-MS) *m/z*: 570 [M+H]⁺

S2. FT-IR table and spectra

Table S1. Infrared absorption of halogen bonding acceptors and complexes.

	Characteristic bands (cm ⁻¹)		
<i>Py1-10</i>	1593	1579	1569
<i>P-Py1-10</i>	1599	1587	1568
<i>M-Py1-10</i>	1601	1589	1568
<i>Py2-S-14</i>	1607	1588	1576
<i>P-Py2-S-14</i>	1605	1591	1575
<i>M-Py2-S-14</i>	1605	1593	1573
<i>Py2-E-14</i>	1605	1583	1577
<i>P-Py2-E-14</i>	1604	1591	1576
<i>M-Py2-E-14</i>	1604	1589	1576

Figure S1. FT-IR comparison of **Py1-10** with its **P** and **M** halogen bonding complexes in neat samples.

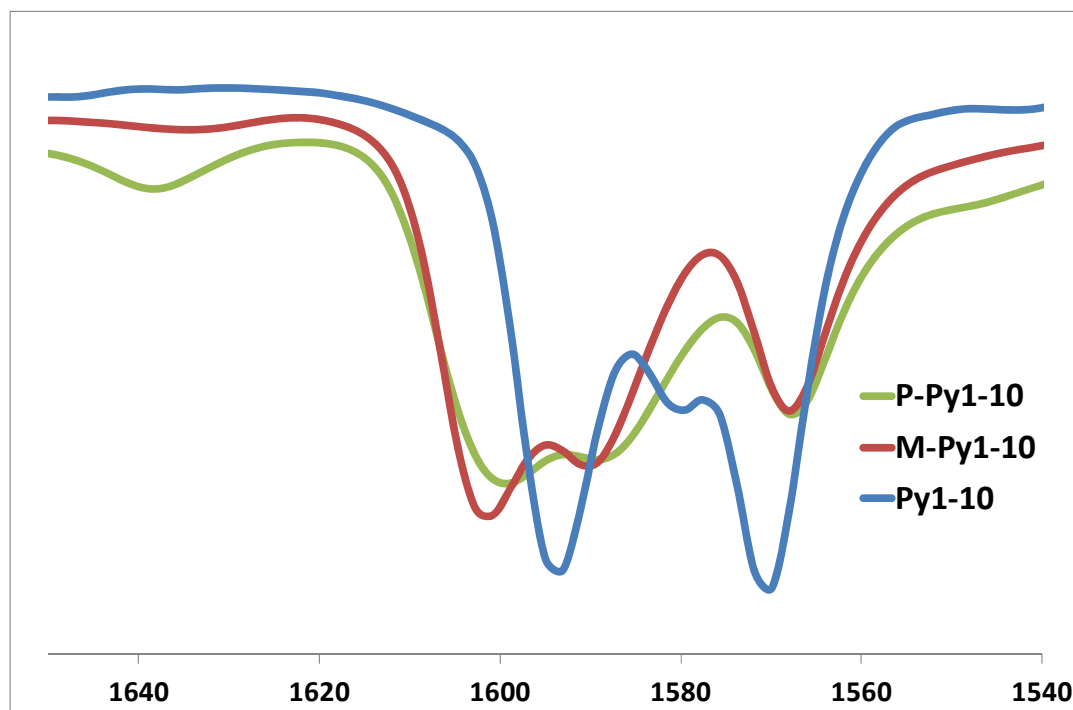


Figure S2. FT-IR comparison of **Py2-S-14** with its **P** and **M** halogen bonding complexes in neat samples.

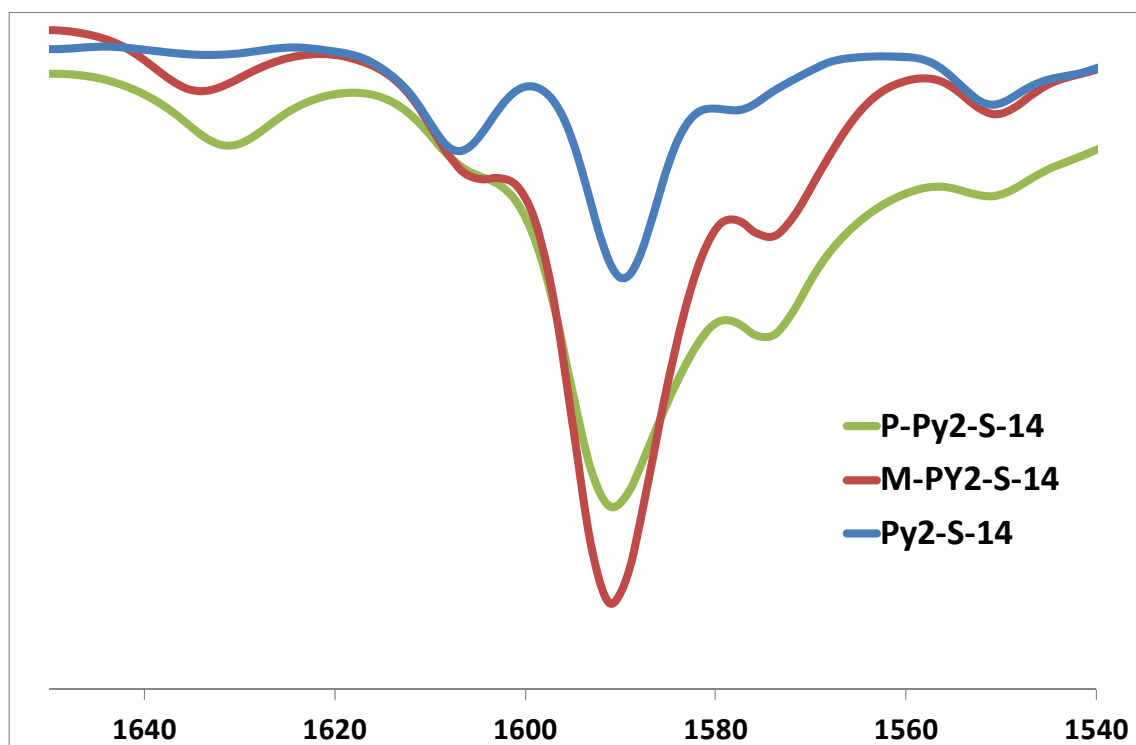


Figure S3. FT-IR comparison of **Py3-S-14** with its **P** and **M** halogen bonding complexes in neat samples.

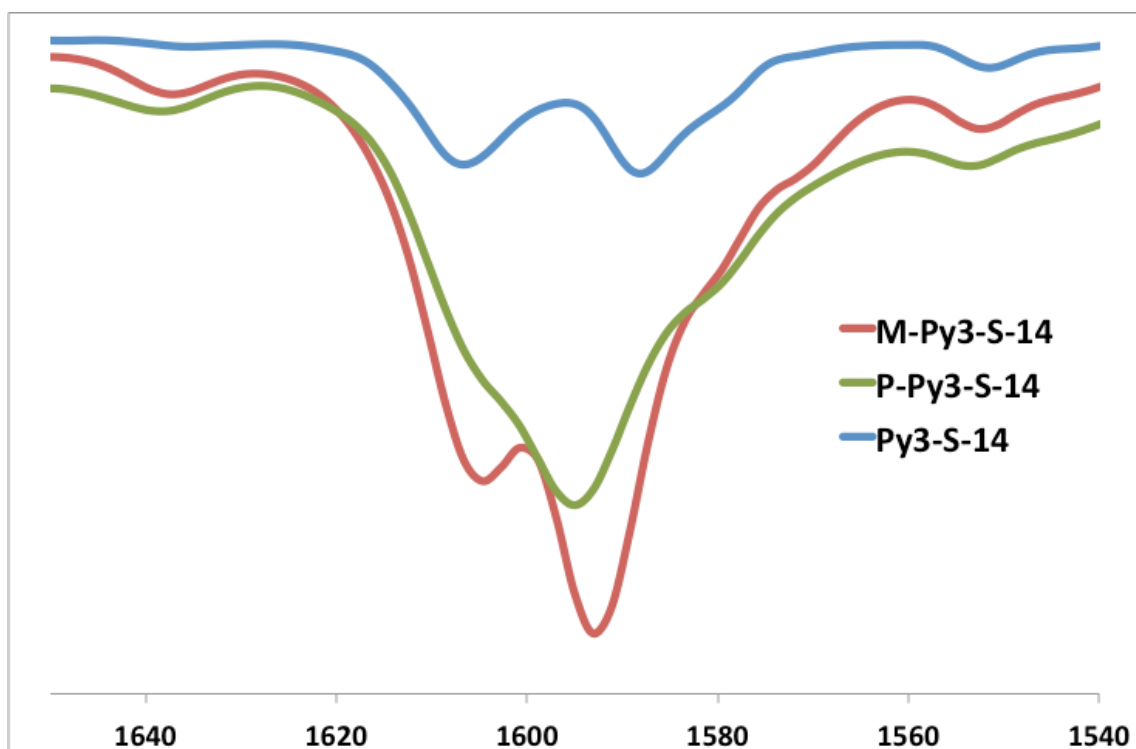


Figure S4. FT-IR comparison of **Py3-S-18** with its **P** and **M** halogen bonding complexes in neat samples.

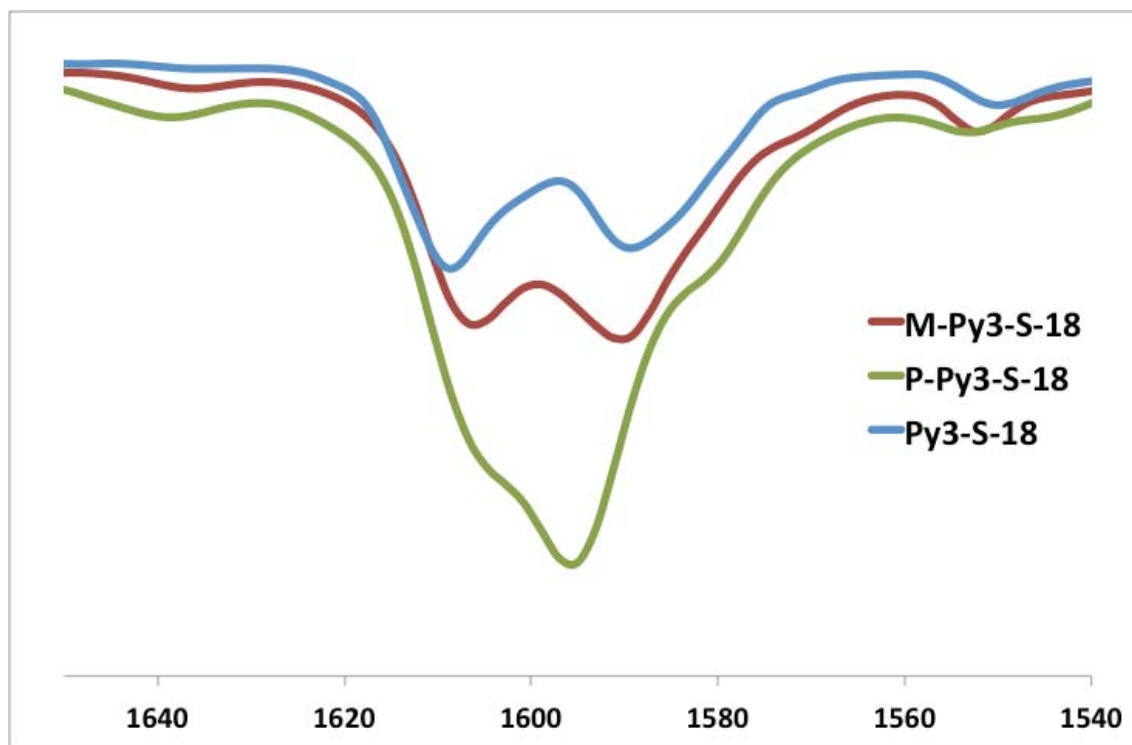
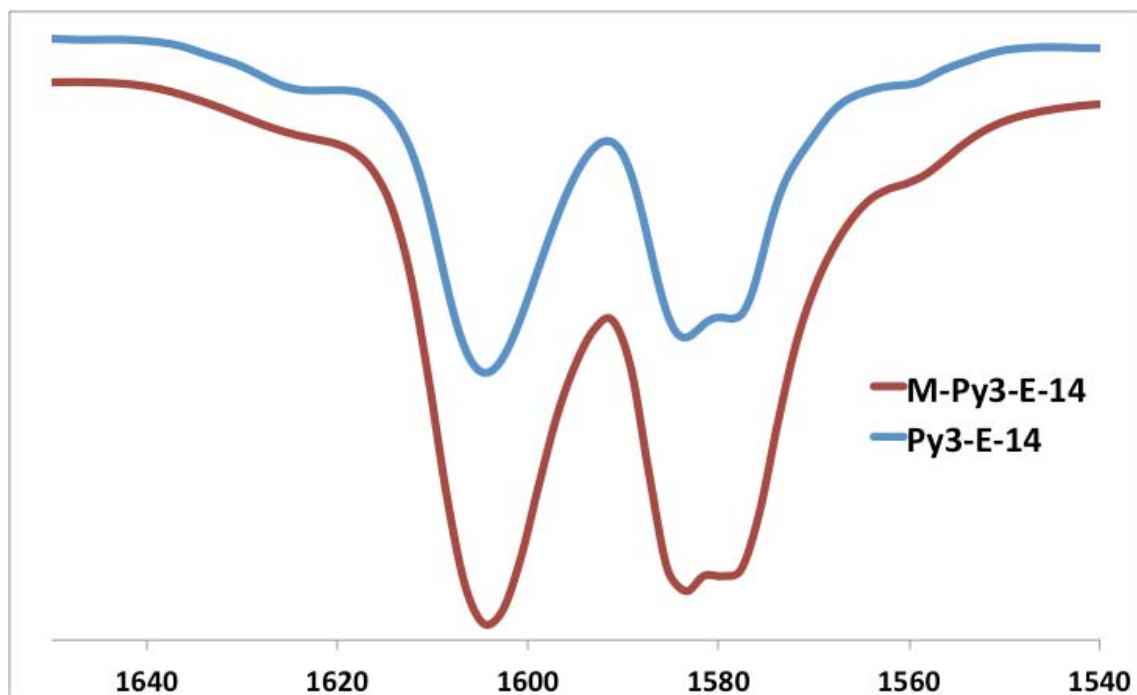


Figure S5. FT-IR comparison of **Py3-E-14** with its **M** halogen bonding complexes in neat samples.



S3. XPS

Table S2. Binding energy of N 1s and I 3d of unbonded ***p*-BIB**, ***m*-BIB** and **Py2-S-14** and X-complexes of series **P** and **M**.

Complexes	N 1s (eV)	ΔBE_{N1s} (eV)	I 3d (eV)	ΔBE_{I3d} (eV)
<i>p</i>-BIB			618.06	
			629.51	
<i>m</i>-BIB			617.96	
			629.41	
Py2-S-14	394.56			
P-Py2-S-14	395.72	1.16	617.96	-0.10
			629.43	-0.08
P-Py3-S-14	395.69	1.13	617.97	-0.09
			629.43	-0.08
P-Py3-S-18	395.68	1.12	617.87	-0.19
			629.31	-0.20
M-Py2-S-14	395.29	0.73	617.60	-0.36
			629.00	-0.41
M-Py3-S-14	395.60	1.04	617.79	-0.17
			629.25	-0.16
M-Py3-S-18	395.70	1.14	617.75	-0.21
			629.24	-0.17
^a $\Delta BE_{N1s} = BE_{N1s}(\text{complex}) - BE_{N1s}(\text{Py2-S-14});$ $\Delta BE_{I3d} = BE_{I3d}(\text{complex}) - BE_{I3d}(\text{BIB})$				

S4. DSC thermograms

Figure S6. DSC thermogram of first heating scans at 10°C/min of (a) **M**, **Py3-S-14** and **M-Py3-S-14** and (b) **M**, **Py3-S-18** and **M-Py3-S-18**.

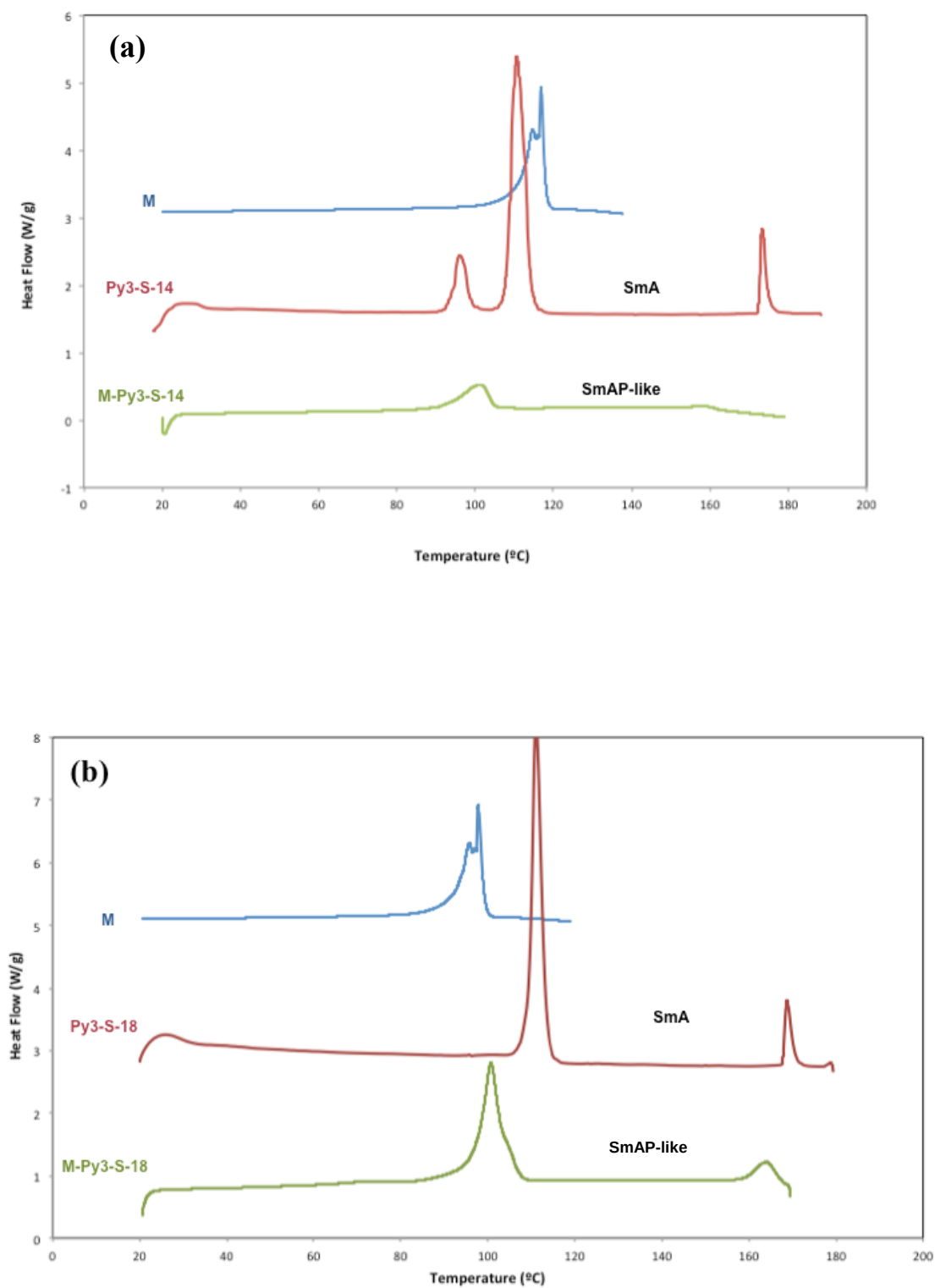
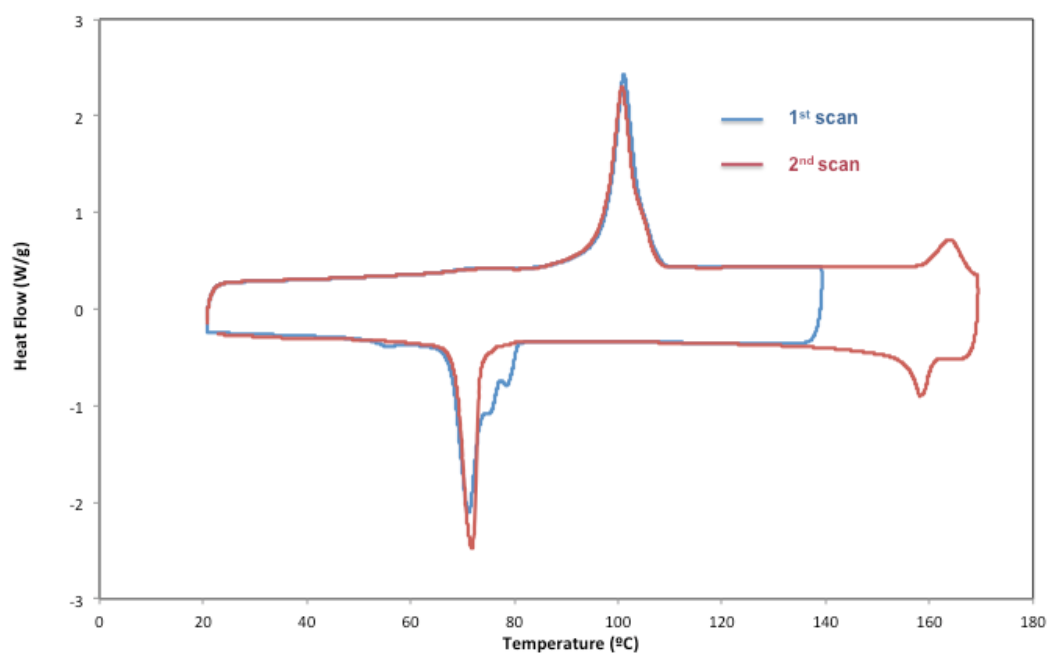


Figure S7. DSC thermogram of XB complex **M-Py3-S18**: on the first heating scan at 10°C/min until 140°C (blue) and on the second heating scan at 10°C until 170°C (red).



S5. XRD diffractograms

Figure S8. X-Ray diffractogram of the XB donor **Py3-E-18** at 140°C in the SmA mesophase. Only one sharp reflection in the low angle region is observed.

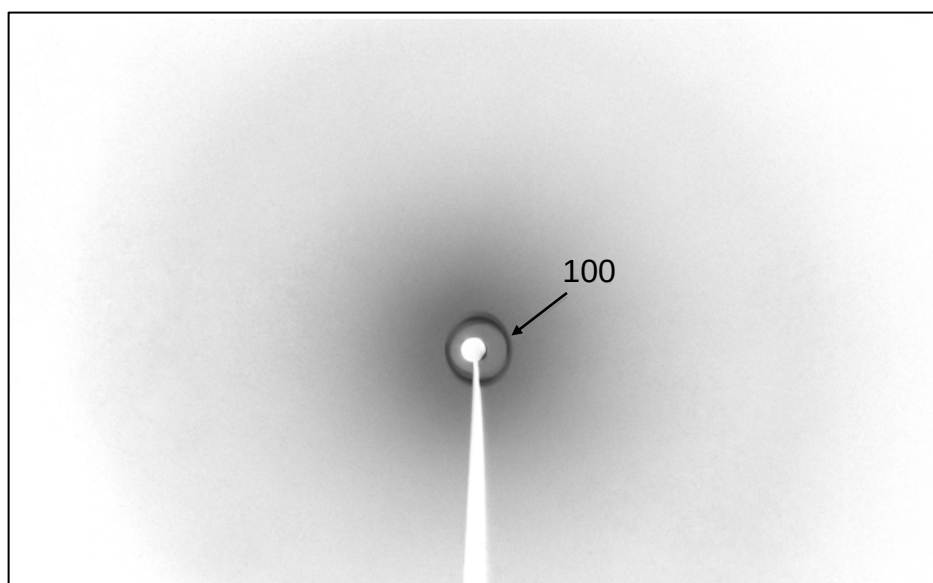


Figure S9. X-Ray diffractogram of the XB complex **M-Py3-E-18** in the SmAP-like mesophase (a) at 120°C and (b) at room temperature after drastic cooling from mesophase temperature. Two sharp reflections in the low angle region are observed.

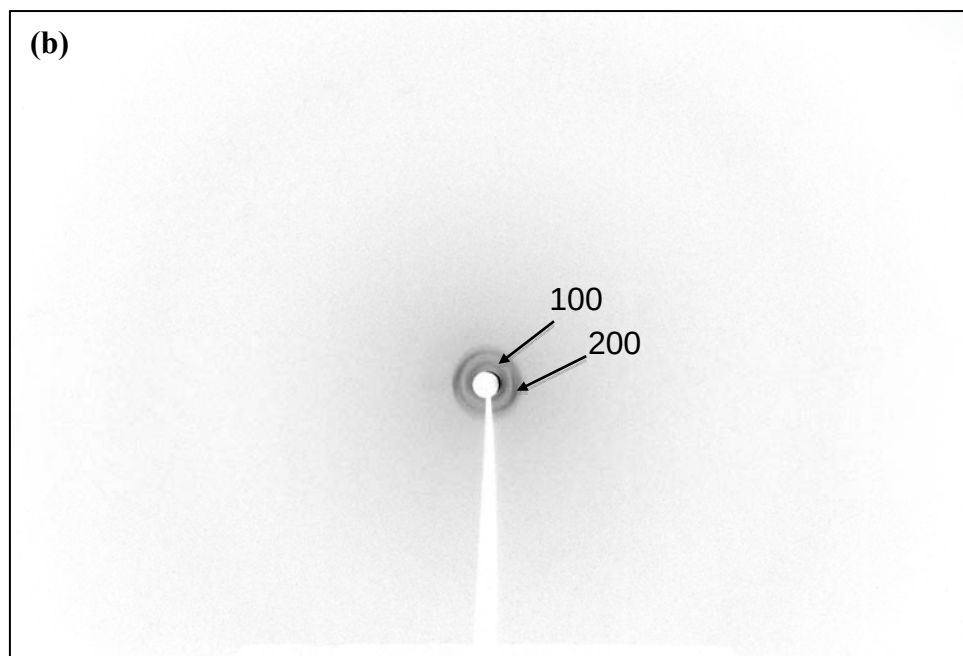
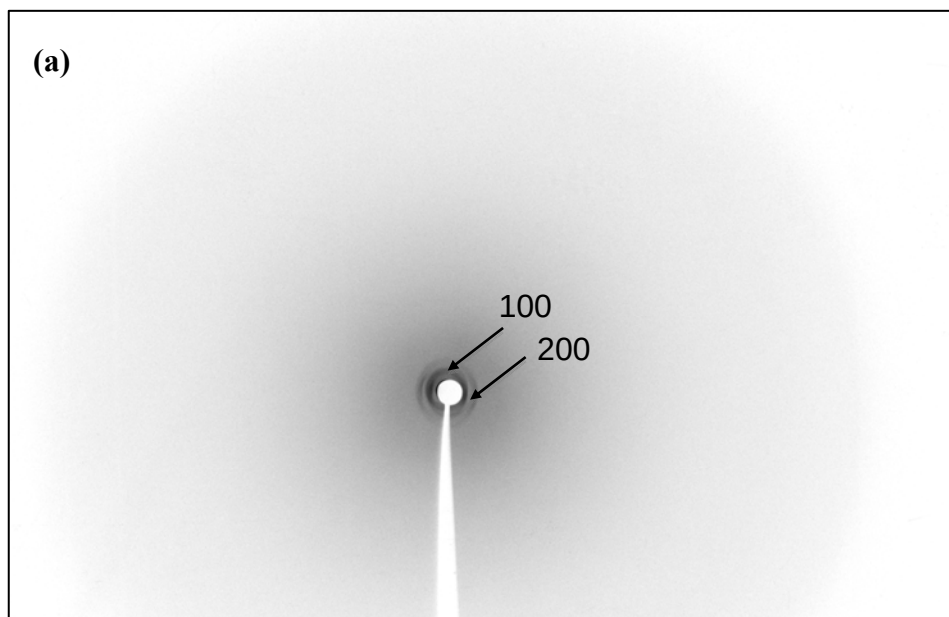
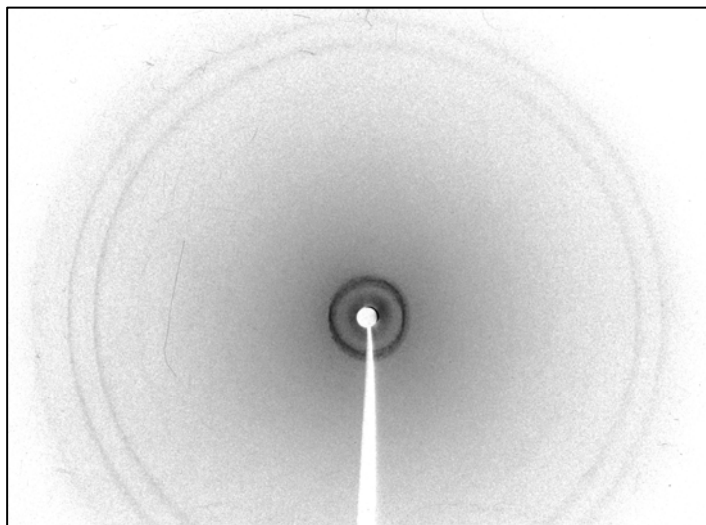


Figure S10. X-Ray diffractogram of the XB complex **P-Py1-10** in the G phase at 95°C.



S6. Crystallography

Final cell parameters were obtained by global refinement of reflections obtained from integration of all the frames data. The structures were solved by direct methods and refined by the full-matrix method based on F^2 using the SHELXTL program.⁶ The non-hydrogen atoms of P-Py1-10 and P-BN-10 were refined anisotropically, the hydrogen atoms were observed in difference electron density maps and refined isotropically. The crystal parameters and basic information relating data collection and structure refinement are summarized in Table S3.

Table S3. Crystallographic data for complexes **P-Py1-10** and **P-BN-10**.

Compound	P-Py1-10	P-BN-10
Empirical formula	C ₄₀ H ₅₄ I ₂ N ₂ O ₂	C ₄₄ H ₅₄ I ₂ N ₂ O ₂
Formula weight	848.65	896.70
Crystal System	Triclinic	Triclinic
a, Å	7.728(3)	8.608(3)
b, Å	9.453(4)	10.221(4)
c, Å	14.800(5)	13.297(5)
α , deg	75.71(3)	97.85(3)
β , deg	84.00(3)	96.79(3)
γ , deg	66.93(4)	113.64(4)
V, Å ³	963.8(6)	1042.2(7)
T, K	150(2)	150(2)
Space group	P-1	P-1
Z	1	1
μ (Mo K α), mm ⁻¹	1.666	1.429
θ range, deg	2.84 / 24.71	2.97 / 26.37
Refl. collected	5810	7425
Uniq reflect / R _{int}	3282 / 0.1458	4262 / 0.1884
R1 ^a /wR2 ^b (I>2 σ)	0.1115 / 0.1637	0.1092 / 0.2913
R1 ^a /wR2 ^b (all data)	0.2226 / 0.2118	0.1476 / 0.2204
Max. shift/esd	0.002	0.016
Residual ρ /e Å ⁻³	-0.690 / 1.081	-1.552 / 0.746

S7. Computational Methods

Quantum chemical calculations were performed using the Gaussian 09⁷ suite programs. Geometry optimizations were carried out in the gas phase with the B98⁸⁻¹⁰ method, employing 6-311G+(d,p)¹¹ basis set for all atoms except iodine for which the DGDZVP¹² basis set was used. Geometry optimizations were carried out without constraints, using the default convergence criteria for the Gaussian software. Vibrational frequency calculations were performed at the same level of the theory as the geometry optimization and the frequency scale factor estimated by Radom *et al*¹³ was used (0.9676). The basis set superposition error (BSSE) for noncovalent complexes was estimated using the counterpoise method of Boys and Bernardi.¹⁴ The natural bond orbital (NBO) analysis¹⁵ using the NBO module containing in Gaussian 09 program were performed on the basis of the minimized structures in order to calculate the NBO charges. The energies of interaction (ΔE_{int}) were calculated by subtracting the electronic energies of the optimized isolated partners ($E_{partner}$) of the electronic energy of the optimized noncovalent complex ($E_{complex}$), in accordance with the following equation:

$$\Delta E_{int} = E_{complex} - \sum E_{partner}$$

The obtained electronic energies of interaction were corrected for scale (0.9884)¹³ zero point differences and for basis set superposition errors.

Calculated gas-phase energy of monomers and complexes optimized with B98/6-311+G(d,p)-DGDZVP and Cartesian coordinates of calculated structures.

Py1-1; Energy (E_{au}), -362.75471 Hartrees				H	-0.85604700	-4.36242400	
C	0.19952300	-1.59574700			0.00000000		
1.14000000				H	-1.63548200	-3.02641700	
C	0.19952300	-0.20175800			0.89447100		
1.20062500				H	-1.63548200	-3.02641700	-
C	0.19707100	0.50990800			0.89447100		
0.00000000				p-BIB; Energy (E_{au}), -14223.39048 Hartrees			
C	0.19952300	-0.20175800	-	C	0.00000000	1.21300000	
1.20062500					0.69401900		
C	0.19952300	-1.59574700	-	C	0.00000000	1.21300000	-
1.14000000					0.69401900		
N	0.19674100	-2.29524000		C	0.00000000	0.00000000	-
0.00000000				1.41011800			
H	0.20616300	-2.17890200		C	0.00000000	-1.21300000	-
2.05797400					0.69401900		
H	0.21655600	0.32110200		C	0.00000000	-1.21300000	
2.15064100					0.69401900		
H	0.21655600	0.32110200	-	C	0.00000000	0.00000000	
2.15064100					1.41011800		
H	0.20616300	-2.17890200	-	H	0.00000000	2.15067400	
2.05797400					1.23815800		
O	0.24793100	1.87865900		H	0.00000000	2.15067400	-
0.00000000					1.23815800		
C	-1.02473500	2.52480200		H	0.00000000	-2.15067400	-
0.00000000					1.23815800		
H	-0.82550700	3.59683100		H	0.00000000	-2.15067400	
0.00000000					1.23815800		
H	-1.60156900	2.25898600	-	C	0.00000000	0.00000000	
0.89443600					2.83577800		
H	-1.60156900	2.25898600		C	0.00000000	0.00000000	-
0.89443600					2.83577800		
BN-1; Energy (E_{au}), -438.94636 Hartrees				C	0.00000000	0.00000000	
C	0.16616800	-0.57561600			4.04759700		
1.21328300				C	0.00000000	0.00000000	-
C	0.16616800	0.81511200			4.04759700		
1.21568500				I	0.00000000	0.00000000	
C	0.16299600	1.51908100			6.04714900		
0.00000000				I	0.00000000	0.00000000	-
C	0.16616800	0.81511200	-		6.04714900		
1.21568500				m-BIB; Energy (E_{au}), -14223.38946 Hartrees			
C	0.16616800	-0.57561600	-	C	0.00000000	0.00000000	
1.21328300					0.72480700		
C	0.16260400	-1.27209900		C	0.00000000	1.21879500	
0.00000000					1.42161300		
H	0.18362300	-1.13244400		C	0.00000000	1.20998500	
2.14390600					2.82955400		
H	0.17433500	1.36217000		C	0.00000000	0.00000000	
2.15175100					3.51959900		
H	0.17433500	1.36217000	-	C	0.00000000	-1.20998500	
2.15175100					2.82955400		
H	0.18362300	-1.13244400	-	C	0.00000000	-1.21879500	
2.14390600					1.42161300		
C	0.16325400	2.95199500		H	0.00000000	0.00000000	-
0.00000000					0.35865400		
N	0.16155800	4.10889300		H	0.00000000	2.15161600	
0.00000000					3.36670900		
O	0.21354500	-2.64104100		H	0.00000000	0.00000000	
0.00000000					4.60445300		
C	-1.05822100	-3.29098900		H	0.00000000	-2.15161600	
0.00000000					3.36670900		

C	0.00000000	-2.45423200		C	-13.92532700	0.89566000	
0.70529400				0.00040700			
C	0.00000000	2.45423200		H	-14.96131600	0.55912600	
0.70529400				0.00053600			
C	0.00000000	-3.50148200		H	-13.73655100	1.49688900	
0.09686300				0.89680700			
C	0.00000000	3.50148200		H	-13.73668600	1.49661000	-
0.09686300				0.89620800			
I	0.00000000	5.22627800	-	C	9.69686700	-0.99377100	
0.91590100				0.00083700			
I	0.00000000	-5.22627800	-	C	9.67217300	1.28958700	-
0.91590100				0.00021400			
P-Py1-1; Energy (E_{au}), -14948.93516 Hartrees							
C	-0.67830800	-1.21989400	-	C	11.09148800	-1.04255000	
0.00089400				0.00052500			
C	0.70983300	-1.20187200	-	H	9.12550900	-1.91895400	
0.00083200				0.00140500			
C	1.41405900	0.01862600	-	C	11.05611600	1.36370900	-
0.00018300				0.00057300			
C	0.67832800	1.22036200		H	9.07598400	2.19833000	-
0.00036400				0.00049400			
C	-0.70984000	1.20233900		C	11.79306100	0.16960100	-
0.00029600				0.00020200			
C	-1.41405200	-0.01811700	-	H	11.59244400	-2.00191200	
0.00031600				0.00083500			
H	-1.21006800	-2.16499700	-	H	11.57208700	2.31656000	-
0.00138100				0.00113600			
H	1.26592200	-2.13287300	-	O	13.13543700	0.28793600	-
0.00127000				0.00058600			
H	1.21004800	2.16548900		C	13.92529200	-0.89585600	-
0.00085200				0.00009800			
H	-1.26588900	2.13336500		H	14.96128700	-0.55934200	-
0.00073300				0.00034100			
C	2.83976200	0.03722900	-	H	13.73665200	-1.49653200	
0.00008400				0.89670000			
C	-2.83975300	-0.03688700	-	H	13.73649500	-1.49735400	-
0.00034600				0.89631400			
C	4.05338500	0.05347200		N	8.98607300	0.13516800	
0.00004900				0.00047900			
C	-4.05337200	-0.05334900	-	N	-8.98608900	-0.13527200	-
0.00032000				0.00006600			
I	6.08066500	0.08541300		M-Py1-1; Energy (E_{au}), -14948.93422 Hartrees			
0.00026300				C	-0.00001100	1.94922900	
I	-6.08064900	-0.08548400	-	0.00005500			
0.00024800				C	1.22074800	2.64386100	-
C	-9.69690800	0.99365300	-	0.00363500			
0.00013400				C	1.21018300	4.05241300	-
C	-9.67216600	-1.28970300		0.00354000			
0.00020900				C	-0.00004000	4.74199800	
C	-11.09152700	1.04240300		0.00034000			
0.00004500				C	-1.21024700	4.05238800	
H	-9.12557100	1.91884800	-	0.00409200			
0.00034400				C	-1.22078300	2.64383200	
C	-11.05611000	-1.36385400		0.00390200			
0.00040400				H	0.00000300	0.86566200	-
H	-9.07596600	-2.19843900		0.00005800			
0.00027100				H	2.15223200	4.58906100	-
C	-11.79307600	-0.16976600		0.00655400			
0.00031500				H	-0.00005100	5.82730000	
H	-11.59251200	2.00175000	-	0.00044400			
0.00002300				H	-2.15230700	4.58901400	
H	-11.57205400	-2.31671900		0.00721800			
0.00062000				C	-2.45903000	1.93162900	
O	-13.13545300	-0.28812200		0.00763000			
0.00053000				C	2.45900700	1.93167600	-
				0.00749300			

C	-3.51695100	1.33789600		H	12.76140000	-1.72460300	
	0.01068000				1.17319800		
C	3.51693100	1.33796200	-	P-BN-1; Energy (E_{au}), -15101.30991 Hartrees			
0.01073300				C	-13.87570700	1.03662600	
I	5.29088900	0.35323800	-		0.15891300		
0.01709000				C	-12.48480600	1.07383700	
I	-5.29091500	0.35316600			0.09965700		
	0.01676000			C	-11.74011100	-0.11287800	
N	-7.85106400	-0.98842300			0.08052200		
	0.02383400			C	-12.41059600	-1.35145900	
C	-8.96166700	-0.28926700	-		0.12158800		
0.21666500				C	-13.79205700	-1.39272600	
C	-7.99740600	-2.29942600			0.18050700		
	0.27641100			C	-14.53693300	-0.20004200	
C	-10.24659600	-0.83343500	-		0.19959800		
0.21936800				H	-14.42826400	1.96731200	
H	-8.82614700	0.77035700	-		0.17243600		
0.42006900				H	-11.97299100	2.02918200	
C	-9.22214600	-2.94787500			0.06814700		
	0.29993000			H	-11.83861200	-2.27233400	
H	-7.08291100	-2.85397100			0.10694400		
	0.46954600			H	-14.32366200	-2.33681400	
C	-10.38321300	-2.20162400			0.21278700		
	0.04683700			O	-15.87816100	-0.34837400	
H	-11.09598200	-0.19464500	-		0.25763500		
0.42389500				C	-16.69863000	0.81268900	
H	-9.29687000	-4.00853700			0.28163100		
	0.50869700			H	-17.72413800	0.44833700	
O	-11.55179600	-2.87159800			0.32880900		
	0.08151500			H	-16.48960800	1.42771500	
C	-12.75690500	-2.15605500	-		1.16438000		
0.16494900				H	-16.56605300	1.41074700	-
H	-13.55798500	-2.88935700	-		0.62715700		
0.08064300				C	-10.31286400	-0.06777800	
H	-12.90616800	-1.36510400			0.02005200		
	0.57856600			N	-9.15782100	-0.03356900	-
H	-12.76182600	-1.72454900	-		0.02859200		
1.17215800				I	-6.06400600	-0.00917600	-
N	7.85115100	-0.98832600	-		0.10588000		
0.02438200				C	-4.05209300	-0.00465300	-
C	8.96173200	-0.28921400			0.13074400		
	0.21639100			C	-2.83902600	-0.00285300	-
C	7.99750900	-2.29934900	-		0.13951800		
0.27683700				C	-1.41346100	-0.00157200	-
C	10.24663000	-0.83343700			0.14508500		
	0.21950100			C	-0.69496300	1.21051100	-
H	8.82620400	0.77043300			0.14605400		
	0.41967600			C	-0.69311300	-1.21257600	-
C	9.22222900	-2.94786200	-		0.14641700		
0.29995800				C	0.69323400	1.21154400	-
H	7.08305100	-2.85386800	-		0.14607900		
0.47021500				H	-1.23972700	2.14814500	-
C	10.38325400	-2.20165400	-		0.14559000		
0.04657200				C	0.69508700	-1.21154200	-
H	11.09597500	-0.19466100			0.14643300		
	0.42423300			H	-1.23648100	-2.15101800	-
H	9.29696900	-4.00854200	-		0.14623500		
0.50863100				C	1.41358300	0.00053800	-
O	11.55181500	-2.87168500	-		0.14511600		
0.08087700				H	1.23660700	2.14998300	-
C	12.75686700	-2.15619800			0.14563800		
	0.16602800			H	1.23984700	-2.14917900	-
H	13.55793700	-2.88955300			0.14626700		
	0.08208400			C	2.83914600	0.00184000	-
H	12.90647700	-1.36531400	-		0.13953500		
0.57749500							

C	4.05221100	0.00376400	-	H	-0.37143900	3.29318300	-
0.13065400				1.06708300			
I	6.06412900	0.00856100	-	C	-1.41588300	5.34036200	
0.10548100				1.45176500			
N	9.15763100	0.03361000	-	H	-1.24413800	6.33337200	
0.02772900				1.85171300			
C	10.31268200	0.06806500		I	3.26805600	3.58676700	-
0.02058500				0.07615000			
C	11.73993400	0.11346100		C	4.19283300	1.81167200	
0.08071300				0.01023200			
C	12.48486500	-1.07309600		C	4.75261500	0.73597800	
0.10033300				0.05730200			
C	12.41018400	1.35219800		C	5.40992100	-0.52893200	
0.12096400				0.10854900			
C	13.87576800	-1.03558300		C	5.94412700	-1.10421900	-
0.15928400				1.06105000			
H	11.97323200	-2.02856000		H	5.85205200	-0.57515600	-
0.06943900				2.00297300			
C	13.79164800	1.39376700		C	5.53431800	-1.22302200	
0.17958200				1.32796100			
H	11.83801600	2.27295200		H	5.12539000	-0.78623500	
0.10592900				2.23218200			
C	14.53676100	0.20123800		I	8.82475700	-7.15130600	
0.19917200				0.38074700			
H	14.42851400	-1.96615200		C	7.91395800	-5.37293700	
0.17318000				0.30165100			
H	14.32307400	2.33797600		C	7.35984700	-4.29630300	
0.21123600				0.25653100			
O	15.87797100	0.34986600		C	6.70589200	-3.03070000	
0.25686400				0.20617700			
C	16.69867000	-0.81102600		C	6.17205000	-2.45479200	
0.28130600				1.37564000			
H	17.72411600	-0.44644900		H	6.26324500	-2.98423200	
0.32811400				2.31733000			
H	16.48993200	-1.42564100		C	6.58201700	-2.33585800	-
1.16440700				1.01292200			
H	16.56604400	-1.40957100	-	H	6.99020800	-2.77312800	-
0.62715600				1.91714600			
Complex p-BN-1; Energy (E_{au}), -15101.30991 Hartrees				I	-10.07635700	-4.29202700	-
I	-5.66010300	0.44286900		1.80155000			
3.61909700				C	-8.20194600	-3.63258000	-
C	-4.32087600	1.62290200		1.57634900			
2.71566200				C	-7.06506100	-3.23624700	-
C	-3.51218900	2.34125700		1.43923600			
2.16899100				C	-5.72627100	-2.77335200	-
C	-2.56448200	3.20290000		1.27800300			
1.54195700				C	-5.39682000	-1.88003100	-
C	-2.33707800	4.49573200		0.24004300			
2.05413500				H	-6.17231800	-1.54199800	
H	-2.88897700	4.82610300		0.43831100			
2.92689000				C	-4.71008000	-3.20445400	-
C	-1.84397400	2.78041500		2.15332300			
0.40805200				H	-4.95625600	-3.89215800	-
H	-2.00682000	1.78487500		2.95461000			
0.00982300				I	1.28348600	-0.36186500	-
I	2.33017500	7.81687100	-	0.41579800			
1.67645700				C	-0.59618700	-1.01687000	-
C	1.04944300	6.54371600	-	0.65185200			
0.81441000				C	-1.73611700	-1.40583900	-
C	0.25021800	5.79105500	-	0.79200100			
0.29848100				C	-3.07612300	-1.86454800	-
C	-0.69567100	4.91844200	-	0.95595900			
0.31698400				C	-3.40587600	-2.75695300	-
C	-0.92449900	3.62722700	-	1.99504300			
0.19652400				H	-2.62887400	-3.09341100	-
				2.67229000			

C	-4.09231700	-1.43319800	-
	0.08093700		
H	-3.84753700	-0.74553800	
	0.72102700		

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