Electronic Supporting Information for

Halogen bonded networks from pyridyl-substituted tetraarylethylenes and diiodotetrafluorobenzenes

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| Bond | Distance (Å) or angle (°) |
|-----------------|---------------------------|
| N5…I1 | 2.796 |
| N6…I7 | 2.896 |
| N7…I6 | 2.878 |
| N8…I8 | 2.884 |
| $C-I1\cdots N5$ | 175.91 |
| C–I7···N6 | 167.85 |
| $C-I6\cdots N7$ | 171.50 |
| $C-I8\cdots N8$ | 173.05 |





Figure S5. Halogen bonding among orthogonally-oriented molecules of **1** in $1 \cdot (1,4-\text{DIB})_2$ (down *c*).









Figure S7. Halogen bonding environment surrounding 1 in $1 \cdot (1,2-DIB)_2$.

| Bond | Distance (Å) or angle (°) |
|-----------------|---------------------------|
| N1…I3 | 2.913 |
| N2…I4 | 3.106 |
| N3…I1 | 2.987 |
| N4…I2 | 2.935 |
| $C-I3\cdots N1$ | 175.24 |
| $C-I4\cdots N2$ | 168.20 |
| $C-I1\cdots N3$ | 167.94 |
| $C-I2\cdots N4$ | 175.76 |









Figure S9. Asymmetric unit in $2 \cdot (1,4-\text{DIB})$.





| Bond | Distance (Å) or angle (°) |
|-----------|---------------------------|
| N4…I2 | 2.917 |
| C–I2···N4 | 166.15 |





Commander Sample ID - File: pigge-fcp11-4b-3-py+1-4-diodo_3-11-2013.raw - Type: 2Th/Th locked - Start: 4.898 * - End: 55.781 * - Step: 0.020 * - Step time: 189. s - Temp.: 25 * C (Room) - Time Started: 0 s - 2-Operations: Displacement 0.250 [Background 1.000,1.000] Import **Figure S12a.** Comparison of calculated powder patterns of **1** (as an EtOAc solvate, red trace)¹ and $1 \cdot (1,2-DIB)$ (blue trace) with observed (black trace) PXRD pattern for $1 \cdot (1,2-DIB)_2$.



¹Kapadia, P. P.; Widen, J. C.; Magnus, M. A.; Swenson, D. C.; Pigge, F. C. *Tetrahedron Lett.* **2011**, *52*, 2519-2522.





Commander Sample ID - File: pigge-fcp11-29-3-py+1-2-diiodo_3-11-2013.raw - Type: 2Th/Th locked - Start: 5.000 ° - End: 55.871 ° - Step: 0.020 ° - Step time: 189. s - Temp.: 25 °C (Room) - Time Started: 0 s - Operations: X Offset - 0.14 | X Offset - 0.034 | Background 1.000,1.000 | Import Y + 30.0 mm - File: 3-pyTPE ElOAc solvate PXRD.raw - Type: 2Th/Th locked - Start: 5.000 ° - End: 50.000 ° - Step time: 0.1 s - Temp.: 25 °C (Room) - Time Started: 0 s - Operations: Range Op. A+B | Import

Figure S13. Comparison of calculated (red trace) and observed (black trace) PXRD patterns for $2 \cdot (1,4-DIB)$.



Commander Sample ID - File: pigge-iodo-pytpe-3.raw - Type: 2Th/Th locked - Start: 10.000 * - End: 50.005 * - Step: 0.020 * - Step time: 945. s - Temp.: 25 *C (Room) - Time Started: 0 s - 2-Theta: 10.000 * - Theta: Operations: Background 1.000.1.000 | Import W + 10.0 mm - File: (pi2104 raw - Type: 2Th/Th locked - Start: 50.000 * - End: 50.000 * - Step: 10.20 * - Step time: 0.1 s - Temp.: 25 *C (Room) - Time Started: 0 s - 2-Theta: 50.000 * - Theta: 2500 * - Chi: 0.00 * - Operations: Y Scale Mul 0.167 | Import



Figure S14. Appearance of $1 \cdot (1,4-\text{DIB})_2$ under ambient light and under irradiation by 366 nm UV light.





