Electronic Supporting Information for

Halogen bonded networks from pyridyl-substituted tetraarylethylenes and diiodotetrafluorobenzenes

F. Christopher Pigge, Pradeep P. Kapadia and Dale C. Swenson

Table of Contents

Figure S1. One unique conformation of **1** in **1**·(1,4-DIB)$_2$ (conformer a).

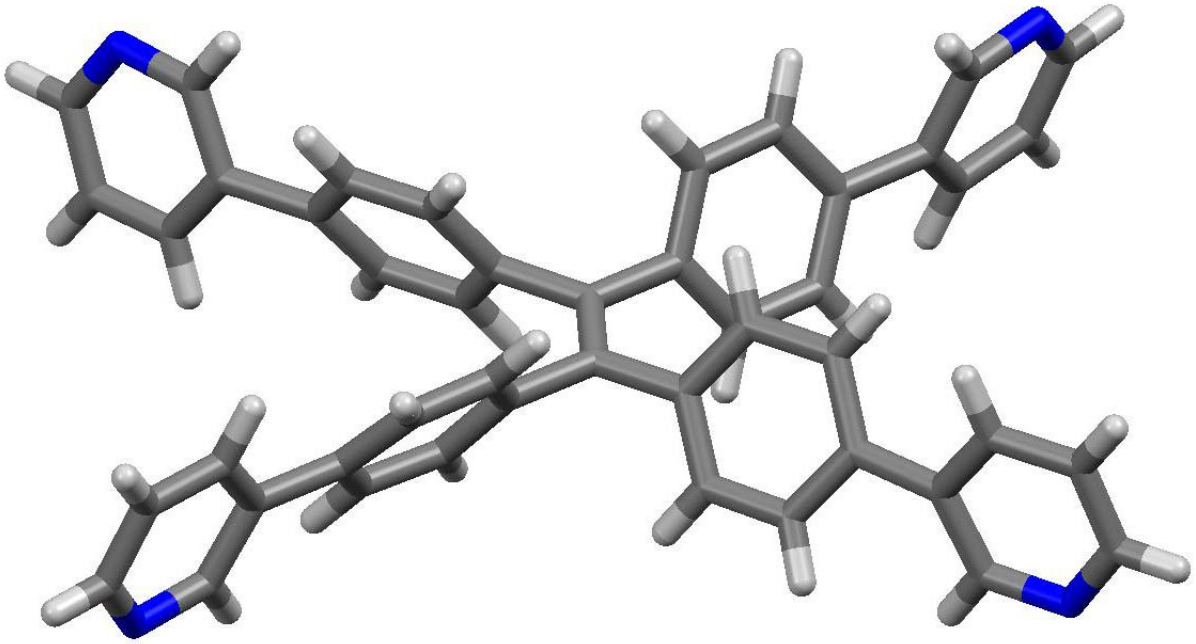


Figure S2. A second unique conformation of **1** in **1**·(1,4-DIB)$_2$ (conformer b).

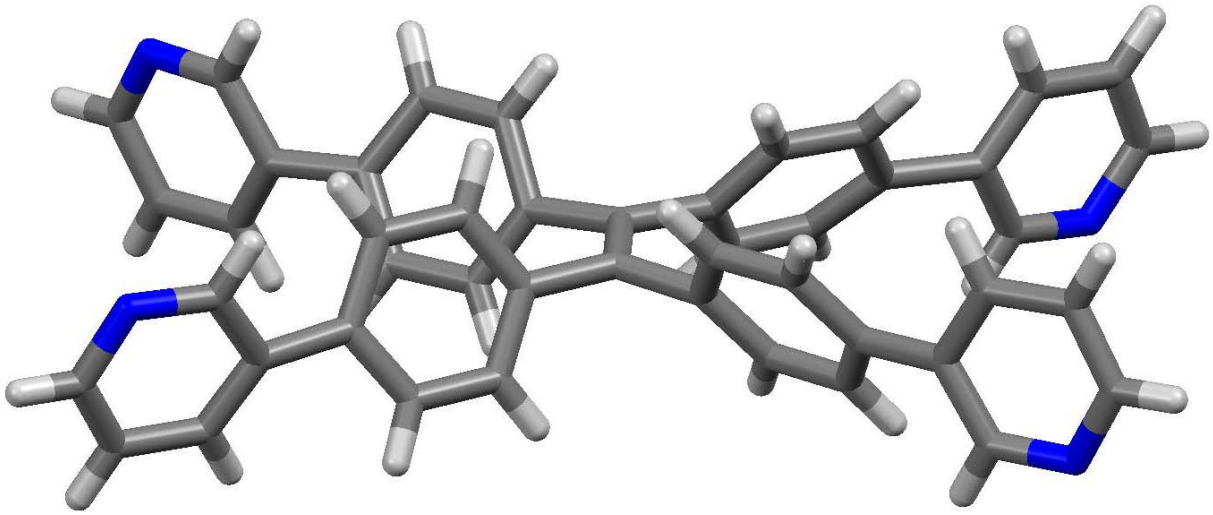
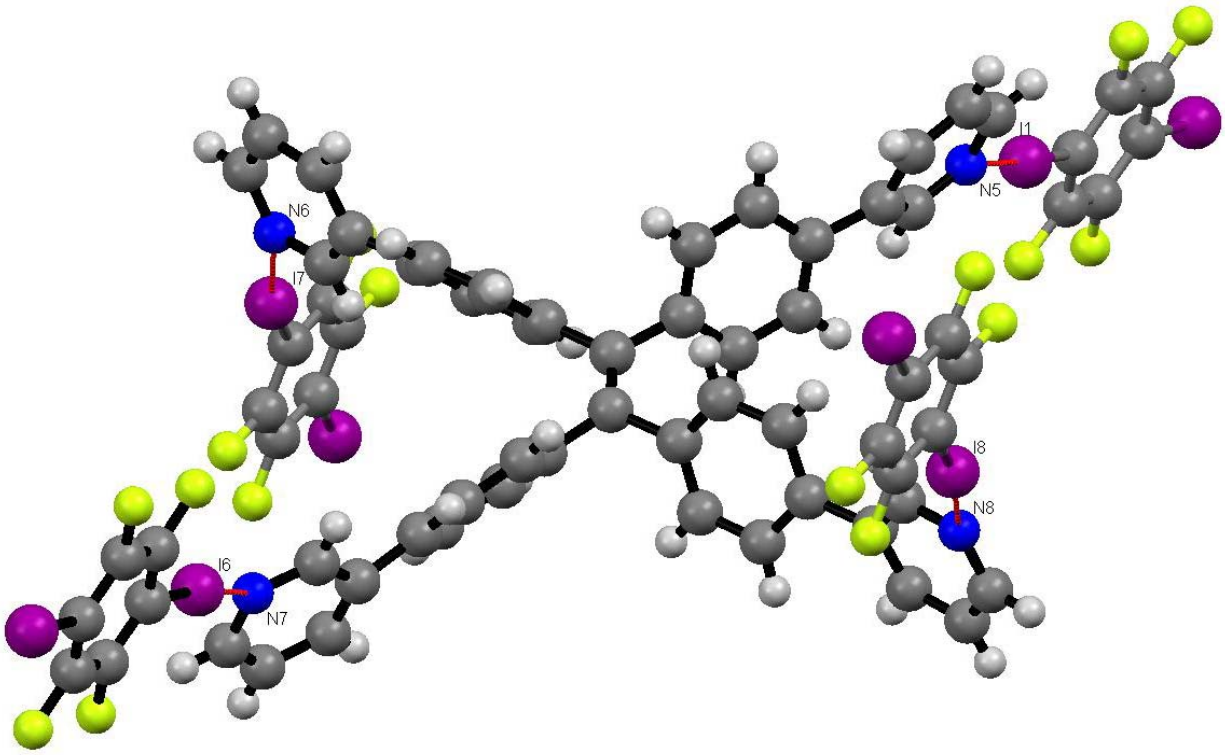
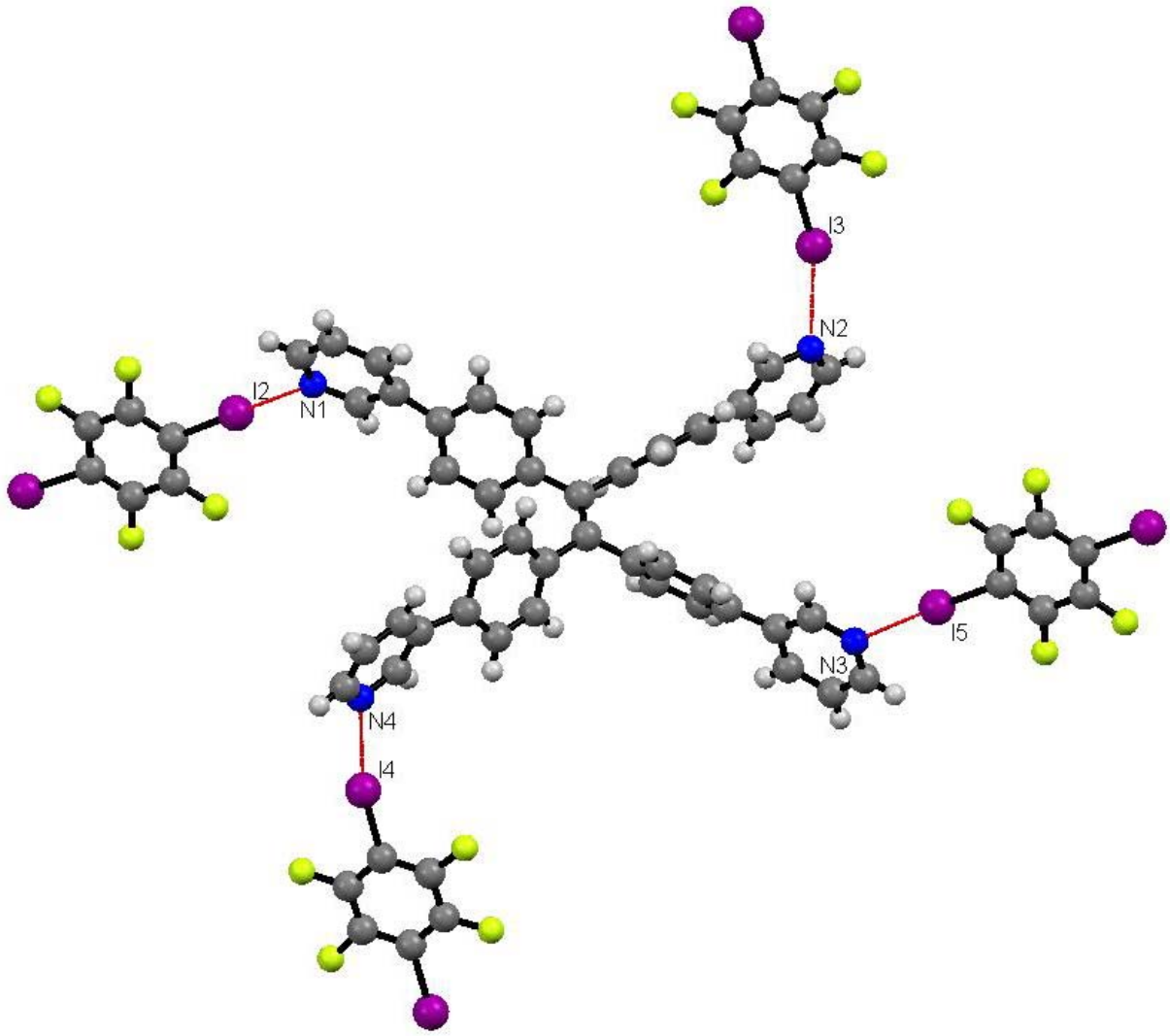


Figure S3. Halogen bonding interactions in **1**·(1,4-DIB)$_2$ (conformer a).



Bond	Distance (Å) or angle (º)
N5···I1	2.796
N6···I7	2.896
N7···I6	2.878
N8···I8	2.884
C–I1···N5	175.91
C–I7···N6	167.85
C–I6···N7	171.50
C–I8···N8	173.05

Figure S4. Halogen bonding interactions in **1**·(1,4-DIB)$_2$ (conformer b).



Bond	Distance (Å) or angle (º)
N1···I2	2.768
N2···I3	3.004
N3···I5	2.814
N4···I4	2.849
C–I2···N1	174.31
C–I3···N2	162.39
C–I5···N3	177.43
C–I4···N4	167.60

Figure S5. Halogen bonding among orthogonally-oriented molecules of **1** in **1**·(1,4-DIB)$_2$ (down *c*).

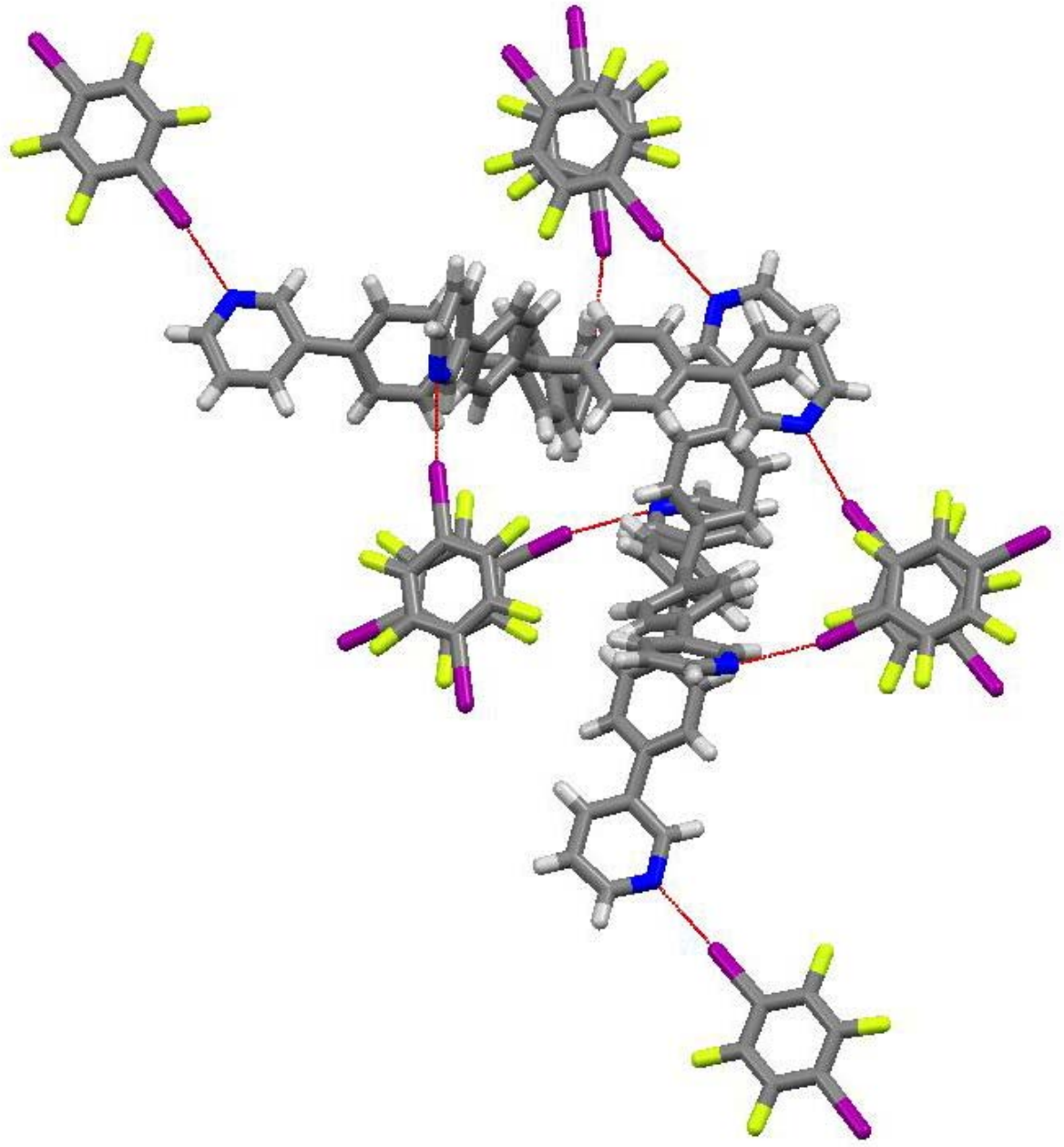


Figure S6. Molecular conformation of **1** in **1**·(1,2-DIB)$_2$.

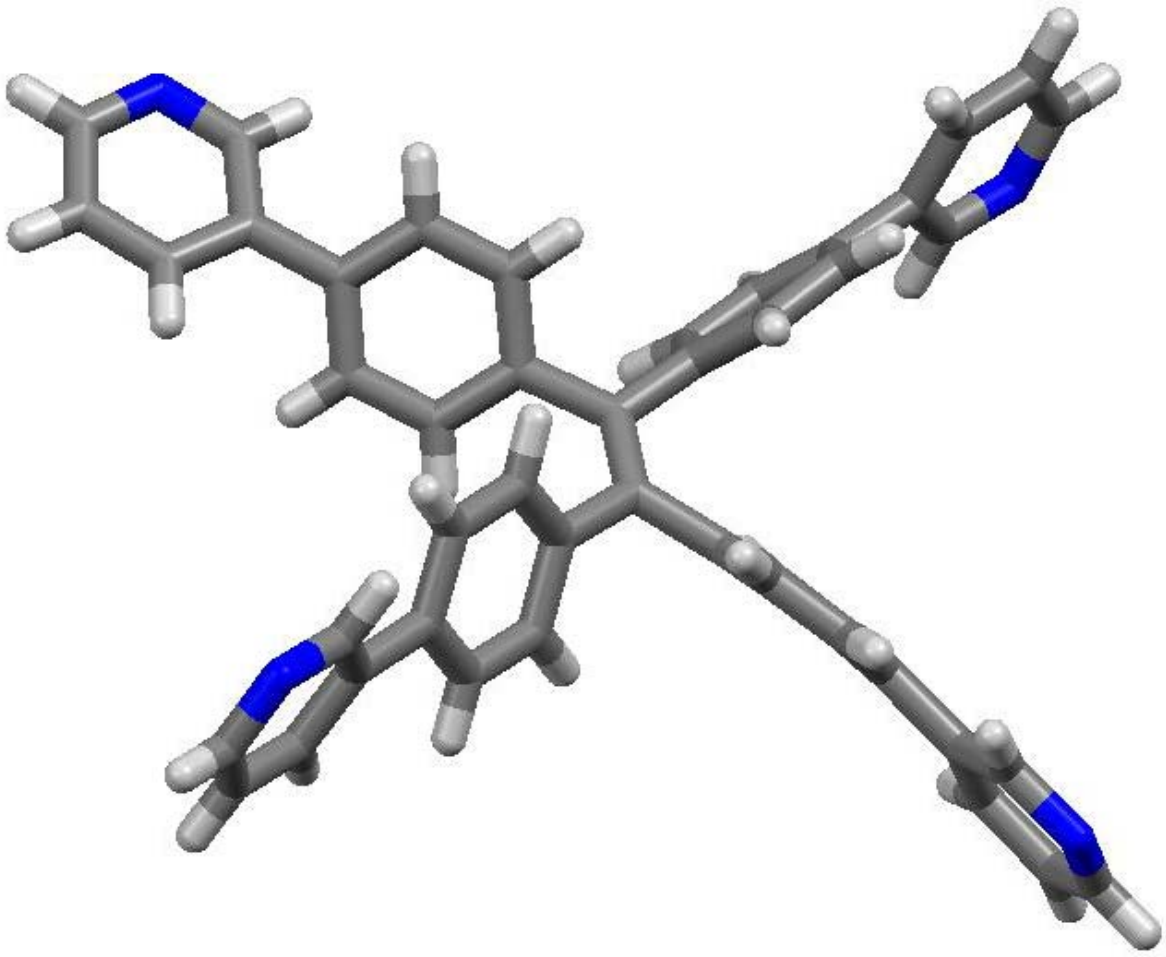
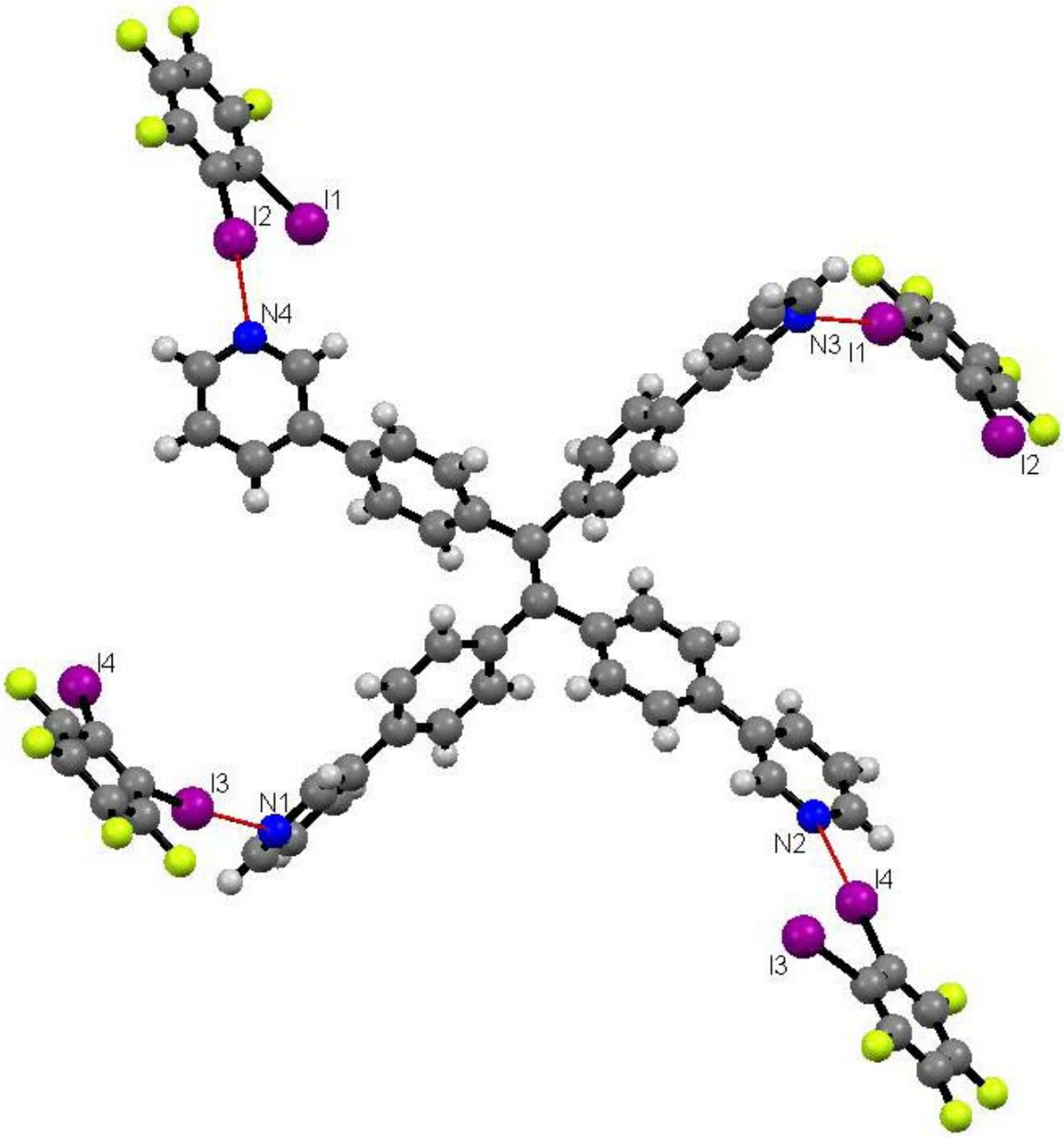
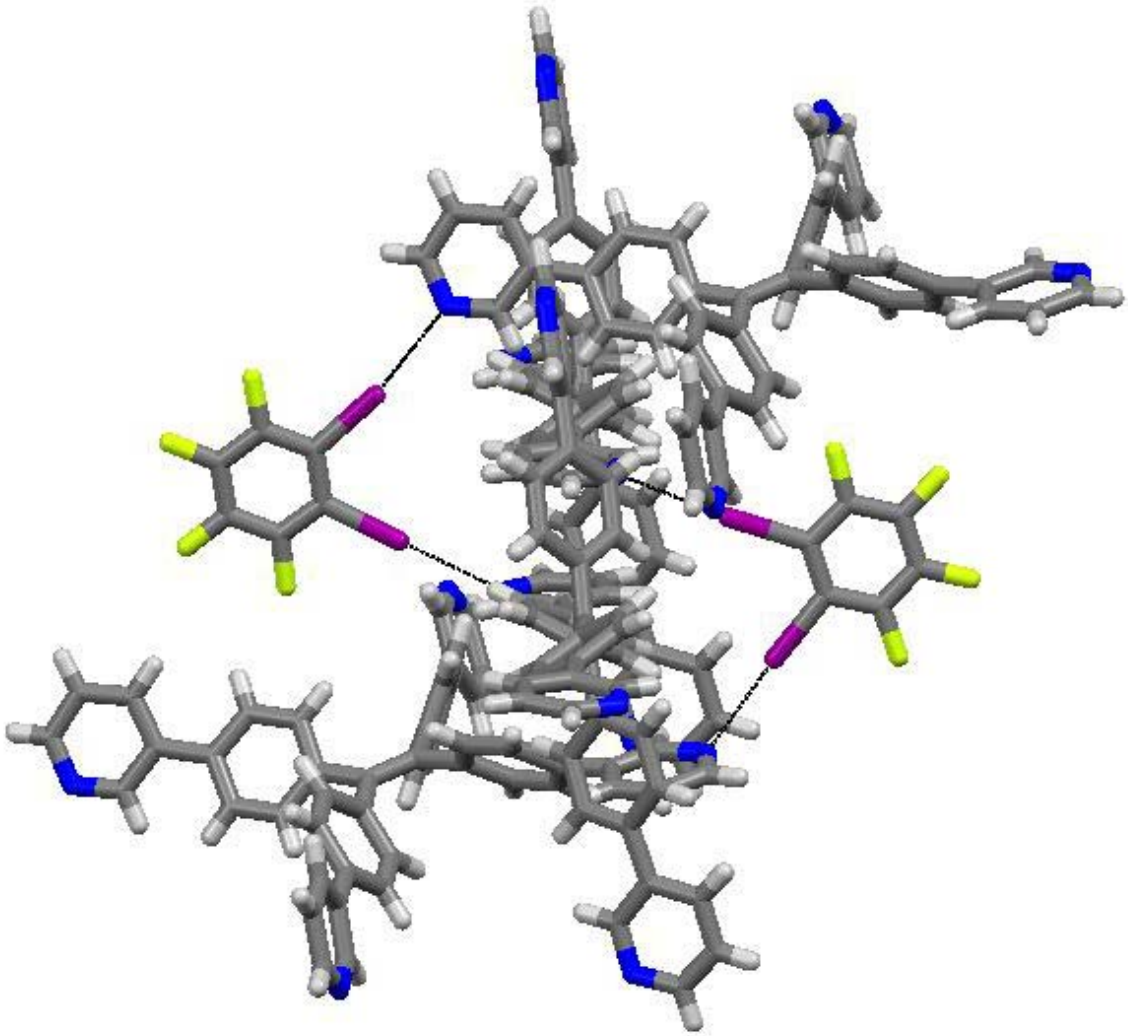


Figure S7. Halogen bonding environment surrounding **1** in **1**·(1,2-DIB)$_2$.



Bond	Distance (Å) or angle (º)
N1···I3	2.913
N2···I4	3.106
N3···I1	2.987
N4···I2	2.935
C–I3···N1	175.24
C–I4···N2	168.20
C–I1···N3	167.94
C–I2···N4	175.76

Figure S8. Two views of halogen bonding network surrounding 1,2-DIB in **1**·(1,2-DIB)$_2$.



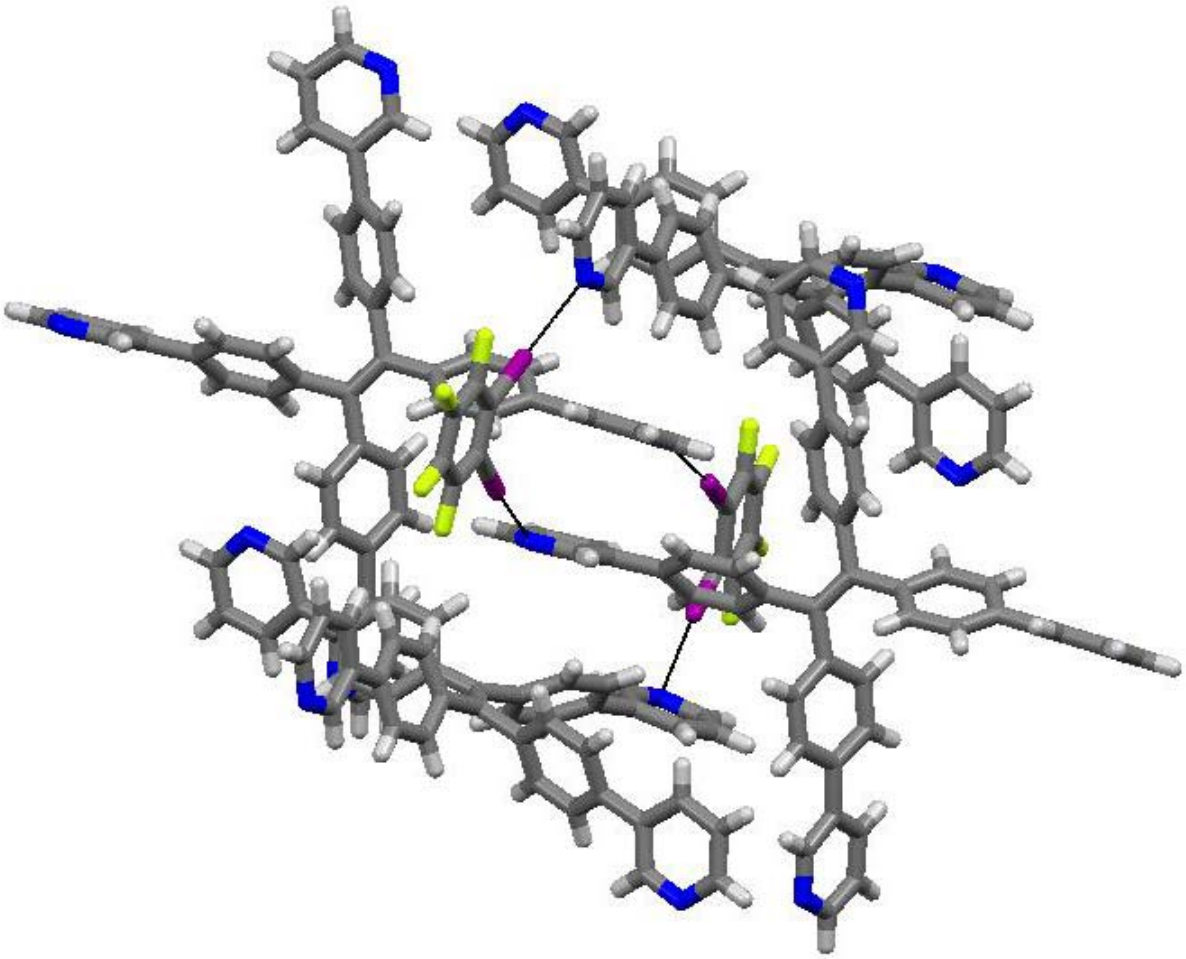


Figure S9. Asymmetric unit in **2**·(1,4-DIB).

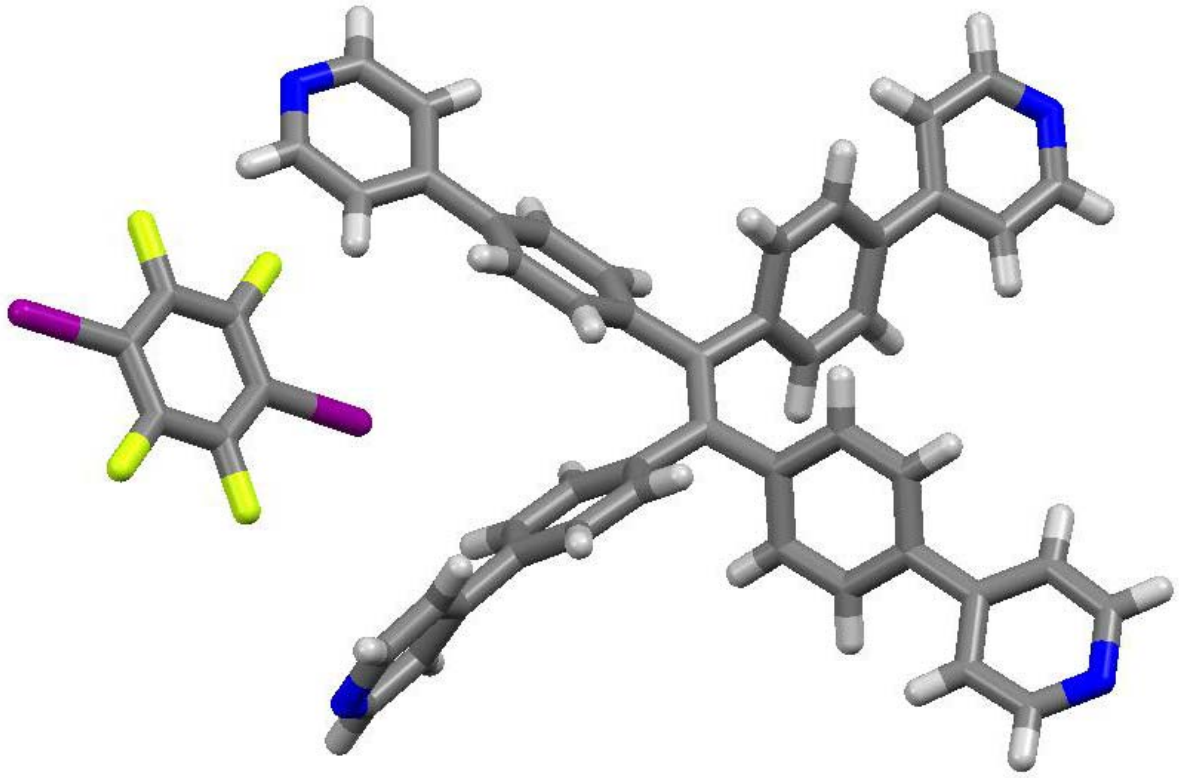
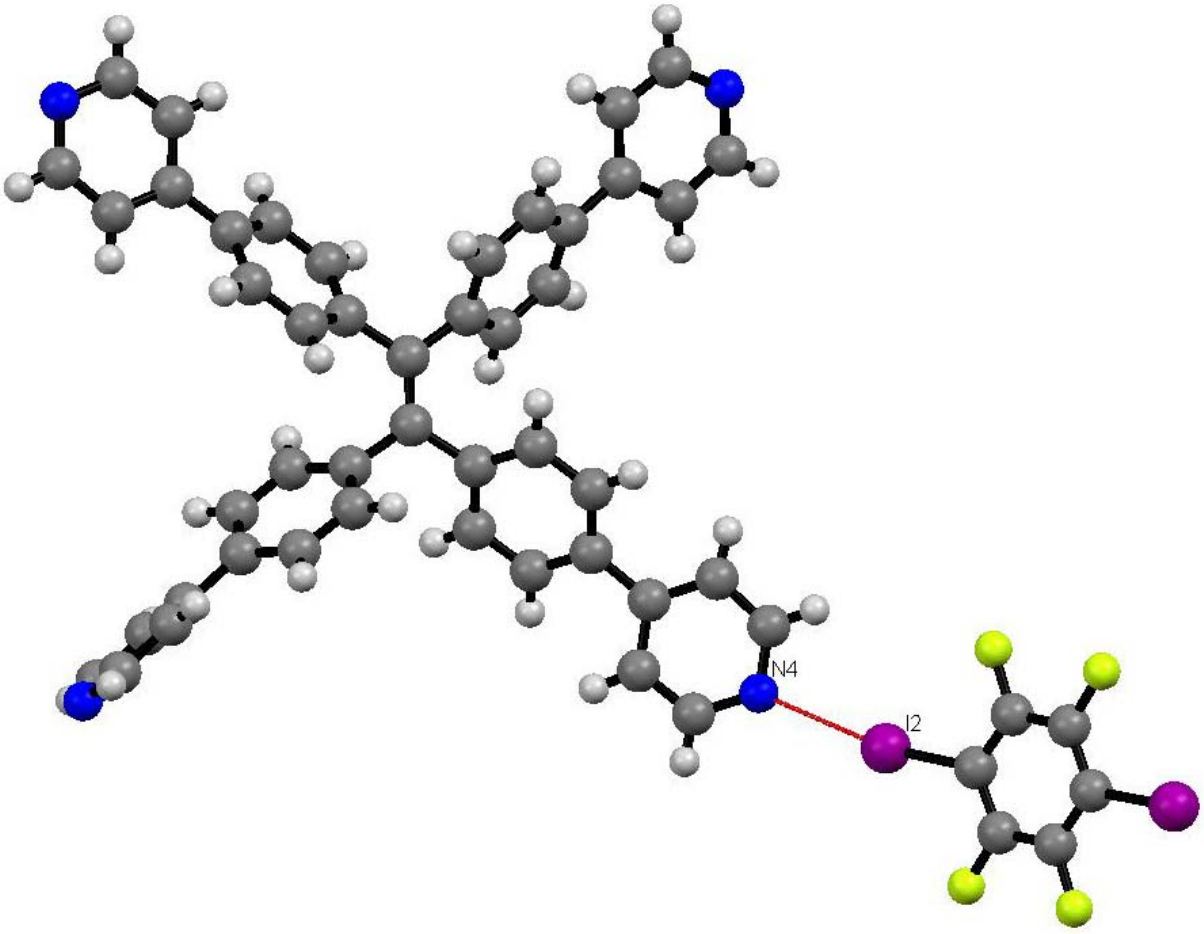


Figure S10. Halogen bonding in **2**·(1,4-DIB).



Bond	Distance (Å) or angle (º)
N4···I2	2.917
C–I2···N4	166.15

Figure S11. Comparison of calculated (red trace) and observed (black trace) PXRD patterns for **1**·(1,4-DIB)$_2$.

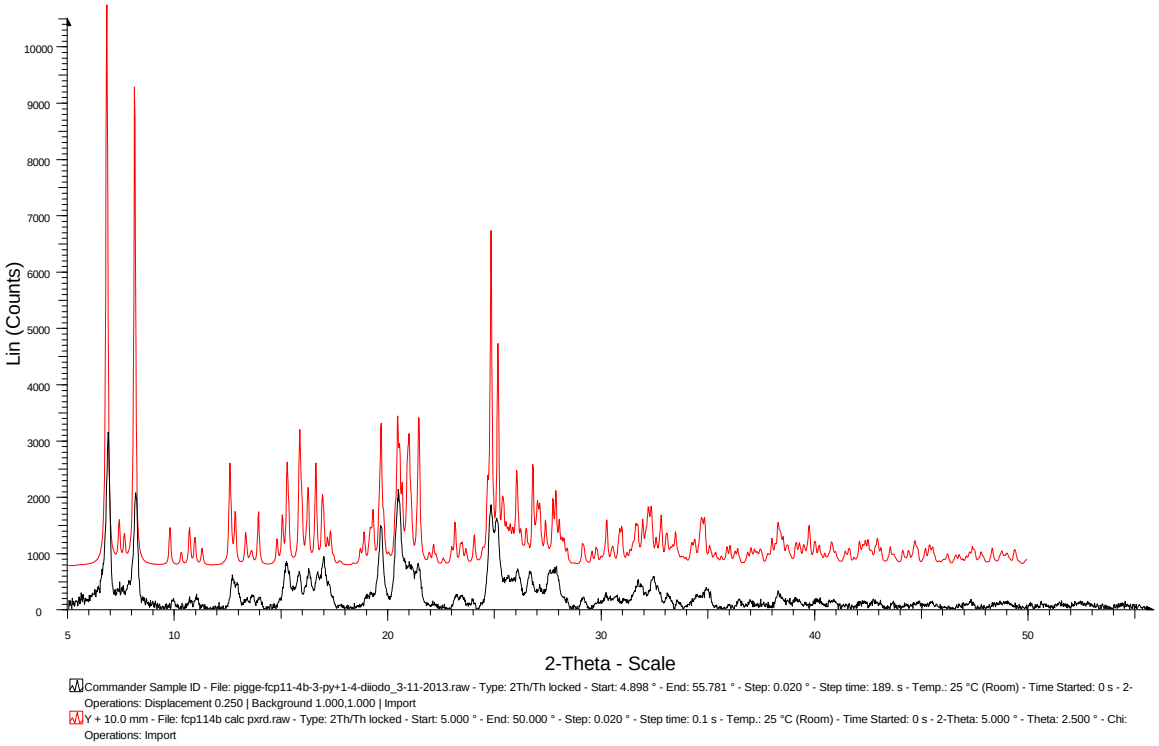
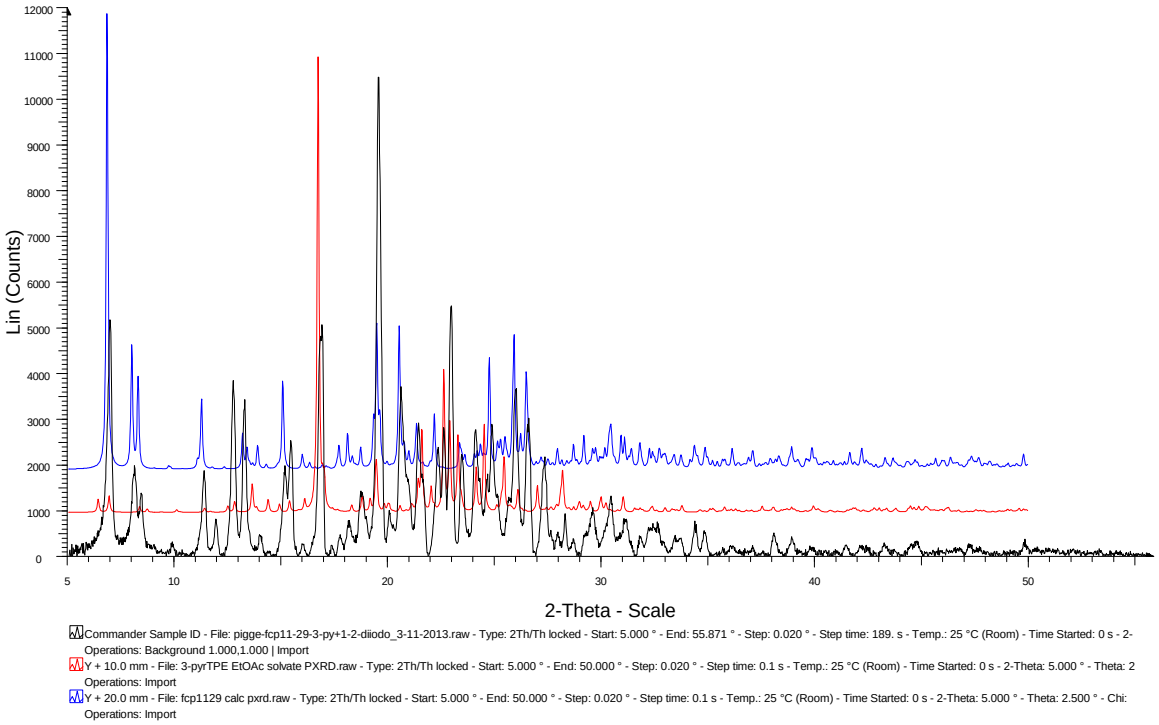


Figure S12a. Comparison of calculated powder patterns of **1** (as an EtOAc solvate, red trace)[1] and **1**·(1,2-DIB) (blue trace) with observed (black trace) PXRD pattern for **1**·$(1,2\text{-DIB})_2$.



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

Figure S12b. Comparison of merged calculated PXRD patterns for **1**·EtOAc and **1**·(1,2-DIB)$_2$ (red trace) with observed PXRD pattern for **1**·(1,2-DIB)$_2$ (black trace).

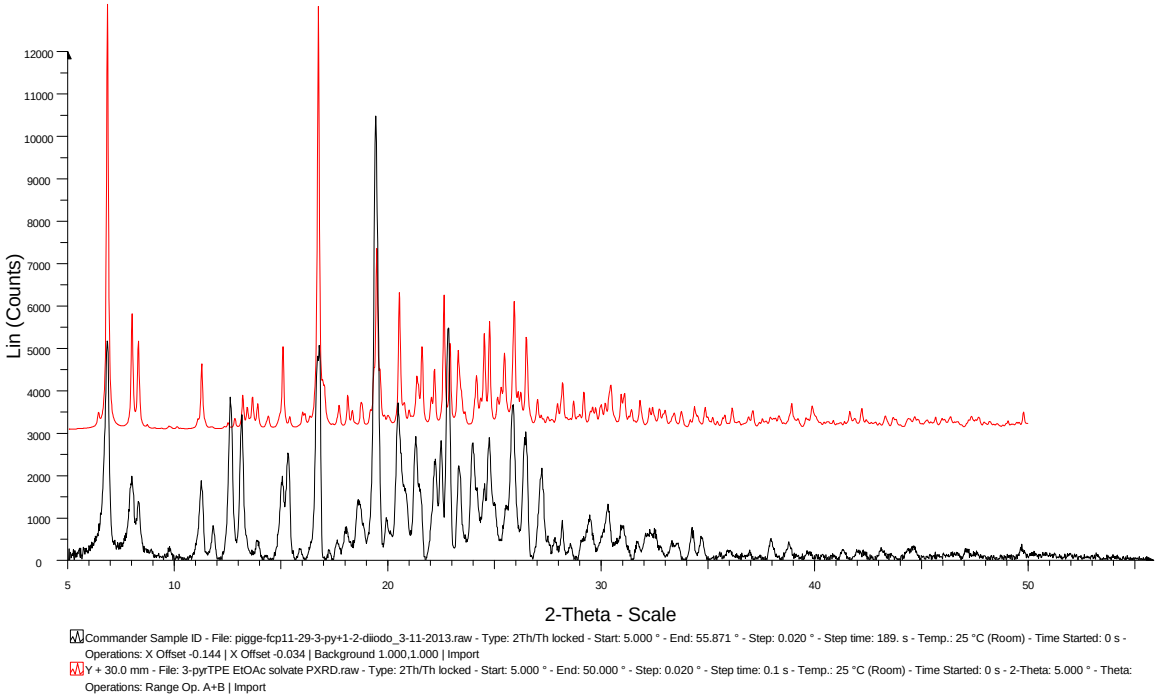


Figure S13. Comparison of calculated (red trace) and observed (black trace) PXRD patterns for **2**·(1,4-DIB).

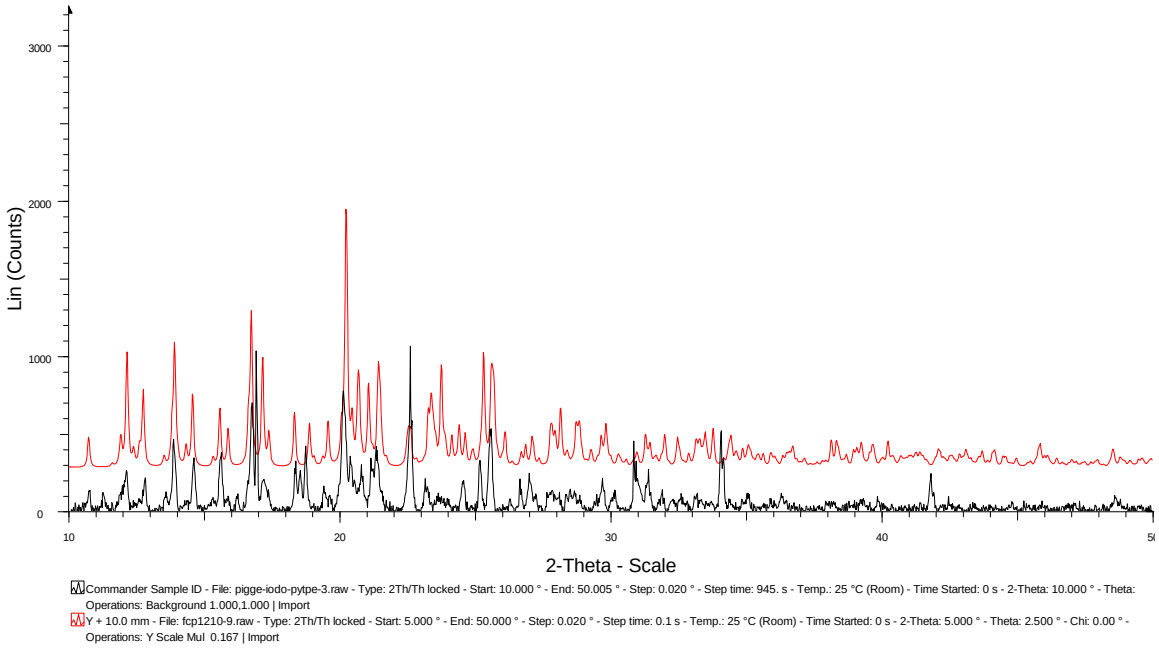


Figure S14. Appearance of **1**·(1,4-DIB)$_2$ under ambient light and under irradiation by 366 nm UV light.

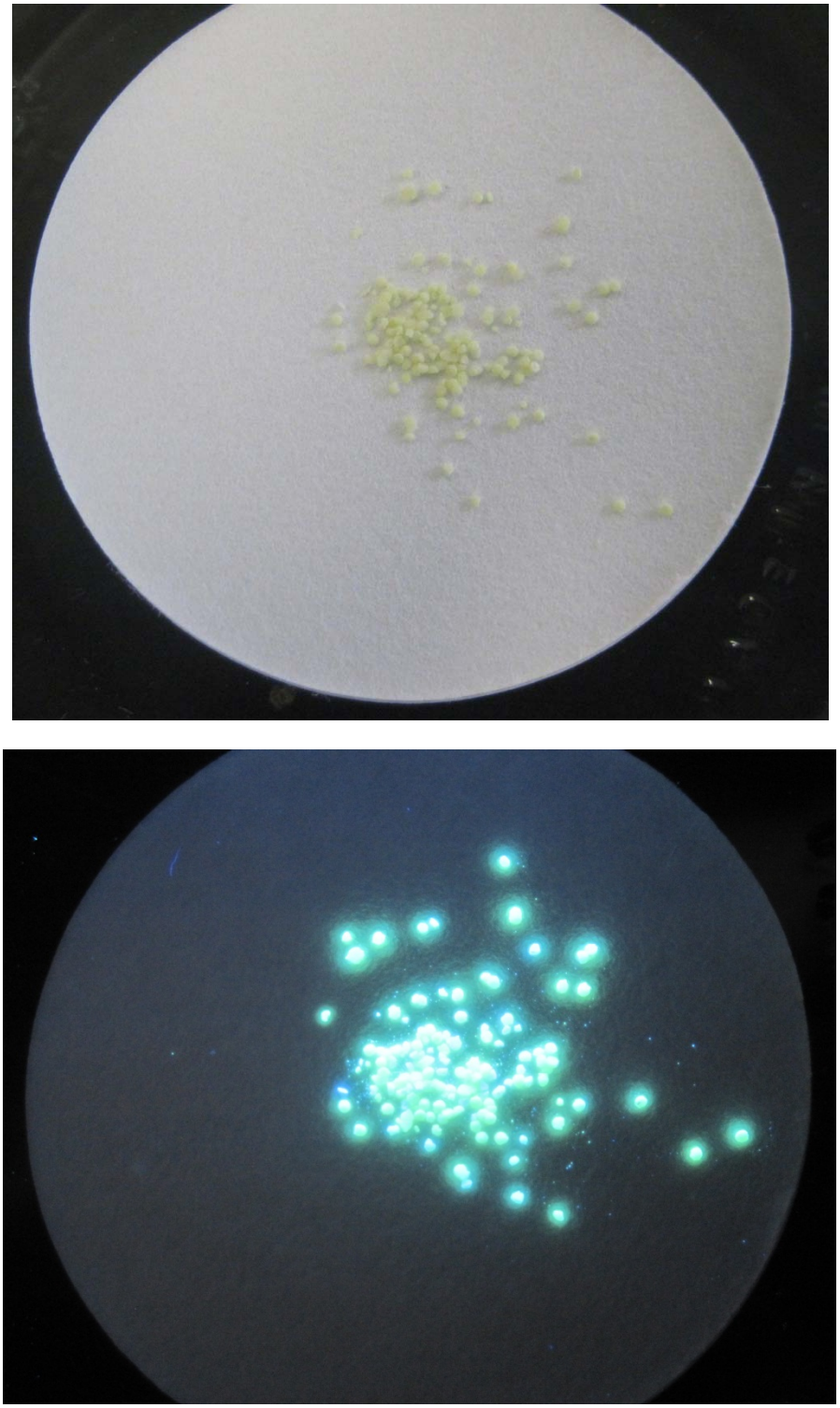


Figure S15. Appearance of **1**·(1,2-DIB)$_2$ under ambient light and under irradiation by 366 nm UV light.