Supplementary Material (ESI) for Chemical Communications

Observation of a two-dimensional halogen-bonded cocrystal at sub-monolayer coverage using synchrotron X-ray diffraction

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Supplementary Data

Experimental details

Based on the estimation of the molecular areas, the number of molecules to cover the graphite surface can be determined. From the number of moles, the appropriate mass of adsorbate can be calculated for the desired coverage and this was then added to the cleaned graphite and sealed under reduced pressue in glass tubes. The reduction of pressure enables us to facilitate equilibration of the samples when annealed elevated temperature before being slowly cooled to room temperature. Disappearance of the adsorbate in the glass tubes indicated when adsorption was complete.

Table S1. Atomic coordinates for the experimentally determined structure of the 2-D (**tfib**)·(**bipy**) cocrystal.[(a)]

Atom type	X_{fract}	Y_{fract}	Z/Å
C1	0.0380540	0.000000	0.000000
C2	0.164783	-0.166382	-0.411097
C3	-0.0179673	0.166382	0.411097
C4	0.235339	-0.166382	-0.411097
C5	0.0525880	0.166382	0.411097
C6	-0.0380540	0.000000	0.000000
C7	0.0179673	-0.166382	0.411097
C8	-0.164783	0.166382	-0.411097
C9	-0.0525880	-0.166382	0.411097
C10	-0.235339	0.166382	-0.411097
N1	0.177942	0.000000	0.000000
N2	-0.177942	0.000000	0.000000
H1	-0.104729	0.280303	0.692571
H2	0.203150	-0.280303	-0.692571
H3	0.0142215	0.280303	0.692571
H4	0.322101	-0.280303	-0.692571
H5	-0.203150	0.280303	-0.692571
H6	0.104729	-0.280303	0.692571
H7	-0.322101	0.280303	-0.692571
H8	-0.0142215	-0.280303	0.692571
C11	0.429445	0.000000	0.000000
C12	0.562251	-0.177354	0.000000
C13	0.367448	0.177354	0.000000
C14	0.632552	-0.177354	0.000000
C15	0.437749	0.177354	0.000000
C16	0.570555	0.000000	0.000000
I1	0.322466	0.000000	0.000000
I2	0.677534	0.000000	0.000000
F1	0.239475	0.348228	0.000000
F2	0.621962	-0.348228	0.000000
F3	0.378038	0.348228	0.000000
F4	0.760525	-0.348228	0.000000

[(a)] only *X* and *Y* coordinates are fractional, the *Z* coordinate is in Ångstroms

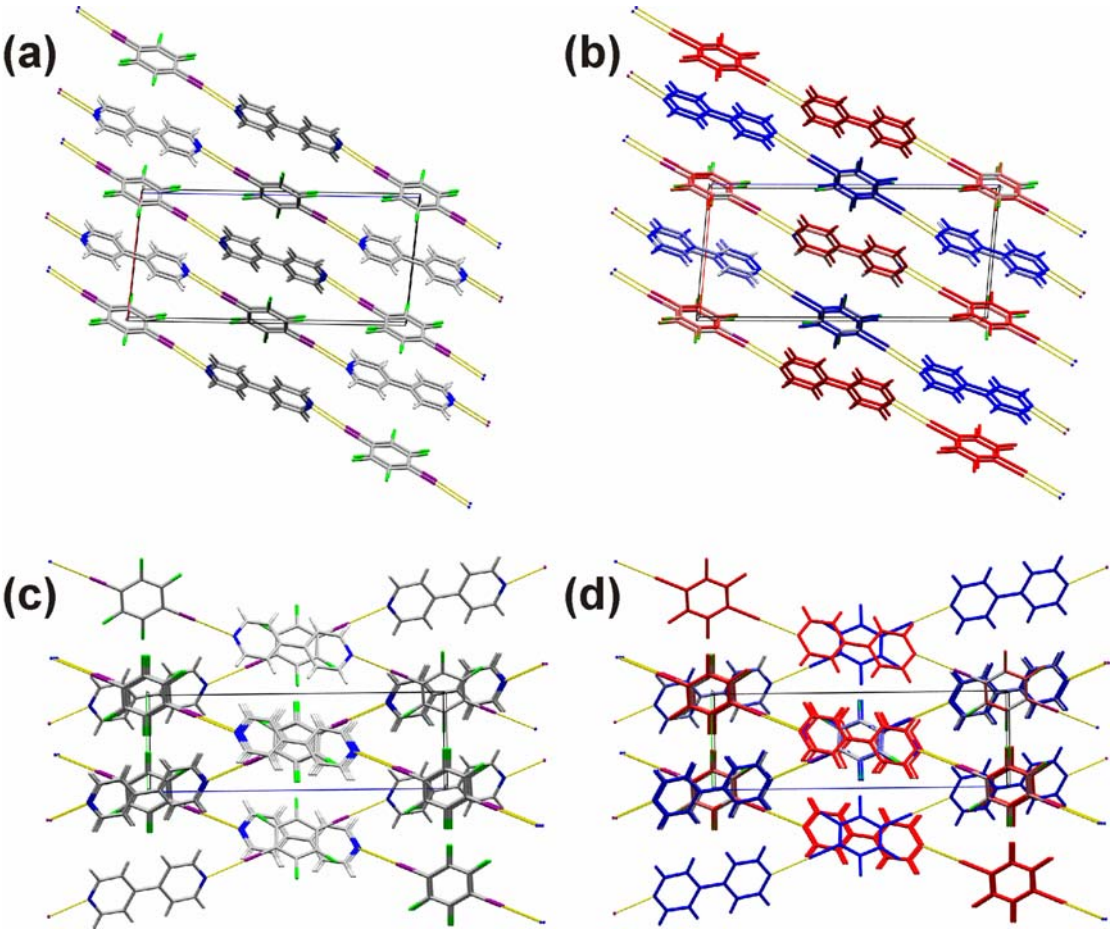

Figure S1. Different views of the (**tfib**)·(**bipy**) bulk cocrystal structure: (a) parallel to the crystallographic *b*-axis and (b) parallel to the *b*-axis with each chain in single color; (b) parallel to the crystallographic *a*-axis and (d) parallel to the *a*-axis with each chain in single color. Whereas the views parallel to the *b*-axis (a and b) suggest a structure similar to that observed for the 2-D cocrystal, the views parallel to the *a*-axis (c and d) reveal that the chains are actually not parallel.