

Supplementary Material (ESI) for Journal of Materials Chemistry  
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**Electronic Supplementary Information for:**

**An extended 9,9'-spirobifluorene based Metal-Organic Framework:  
synthesis, structure analysis and gas sorption properties.**

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SI-1.  $^1\text{H}$  NMR spectra of **3** and **L**

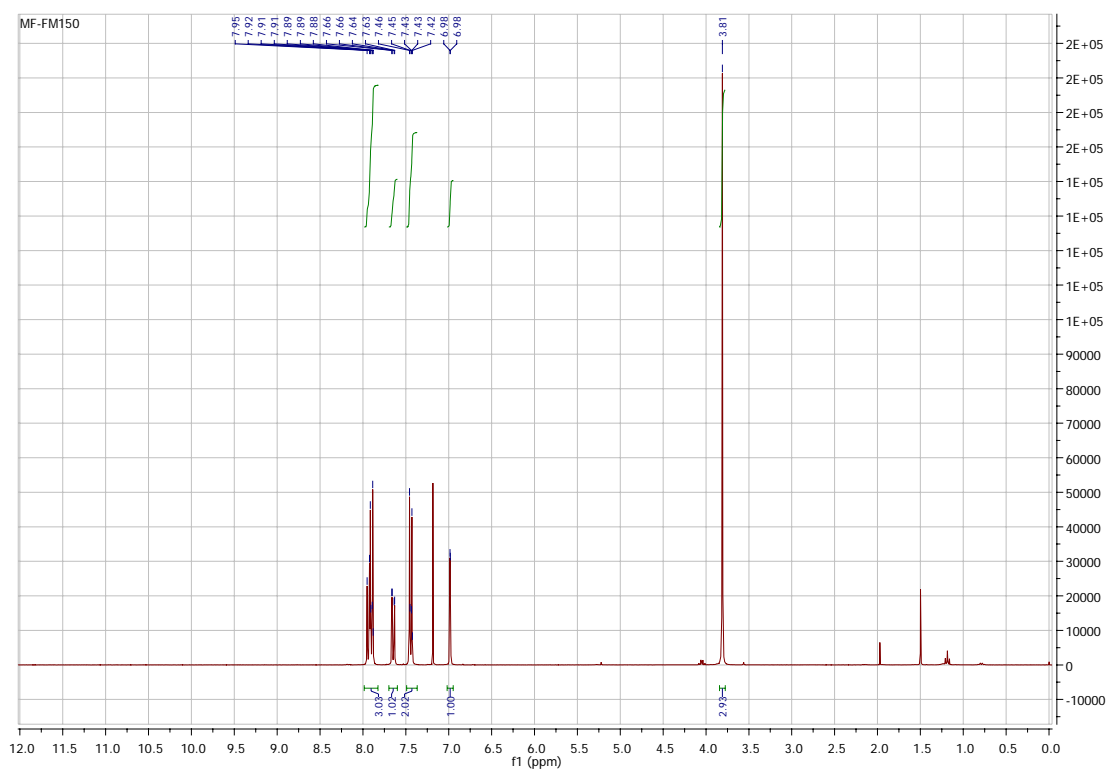


Figure S1.  $^1\text{H}$  NMR spectra of **3** in  $\text{CDCl}_3$

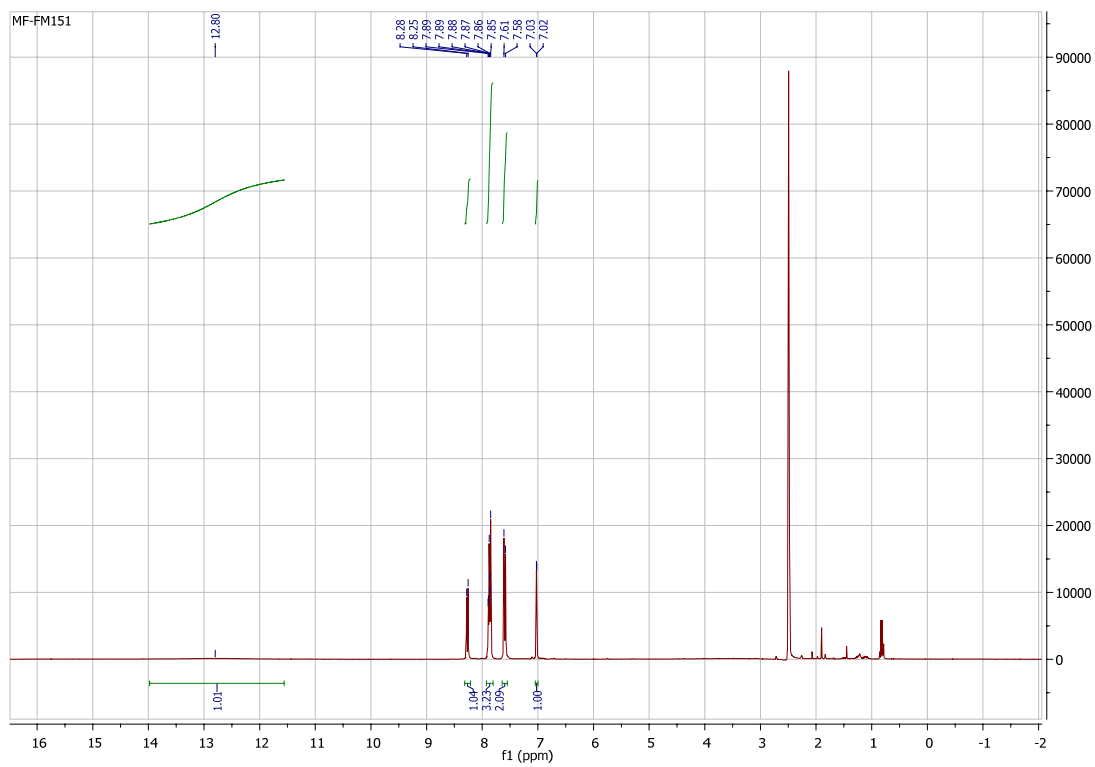


Figure S2.  $^1\text{H}$  NMR spectra of **L** in  $[\text{D}_6]\text{DMSO}$

SI-2.  $^{13}\text{C}$  NMR spectra of **3** and **L**

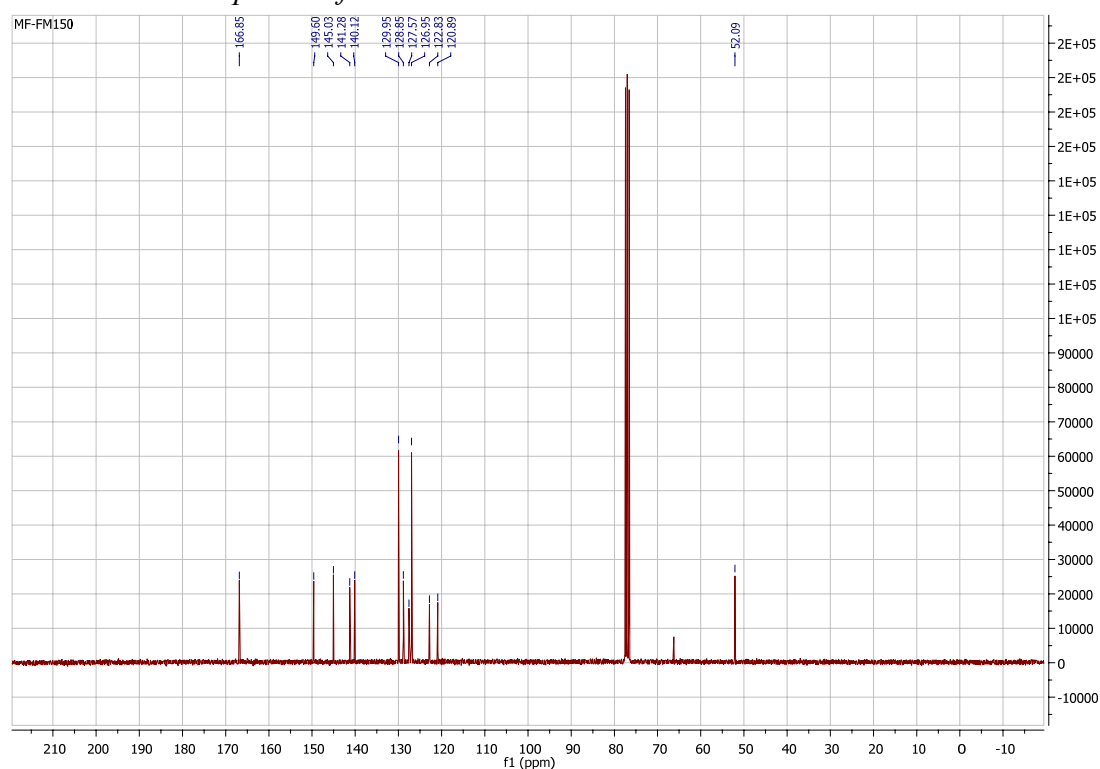


Figure S3.  $^{13}\text{C}$  NMR spectra of **3** in  $\text{CDCl}_3$

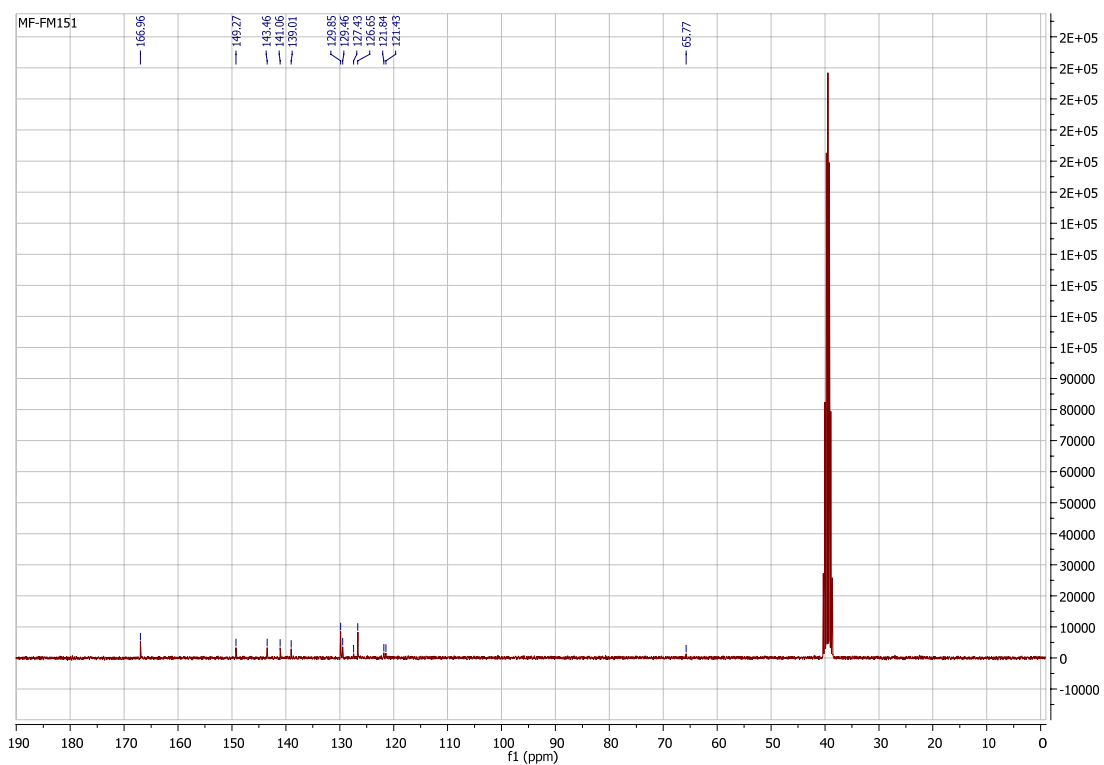


Figure S4.  $^{13}\text{C}$  NMR spectra of **L** in  $[\text{D}_6]\text{DMSO}$

**SI-3.** IR transmission spectra of **3**, **L**, **SBF-Cu**, and **SBF-Cu\_act**

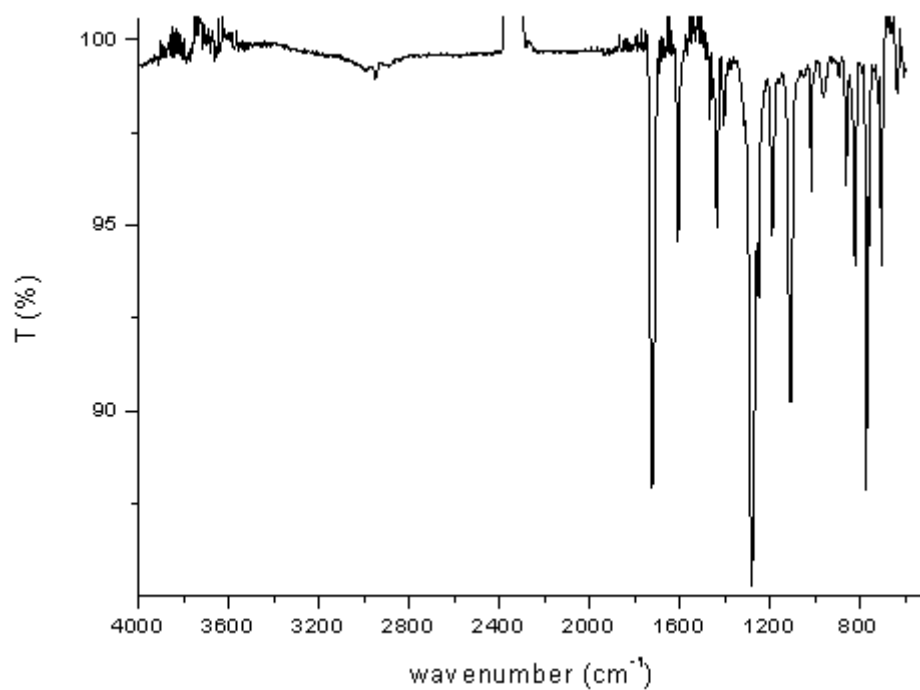


Figure S5. IR transmission spectra of **3**

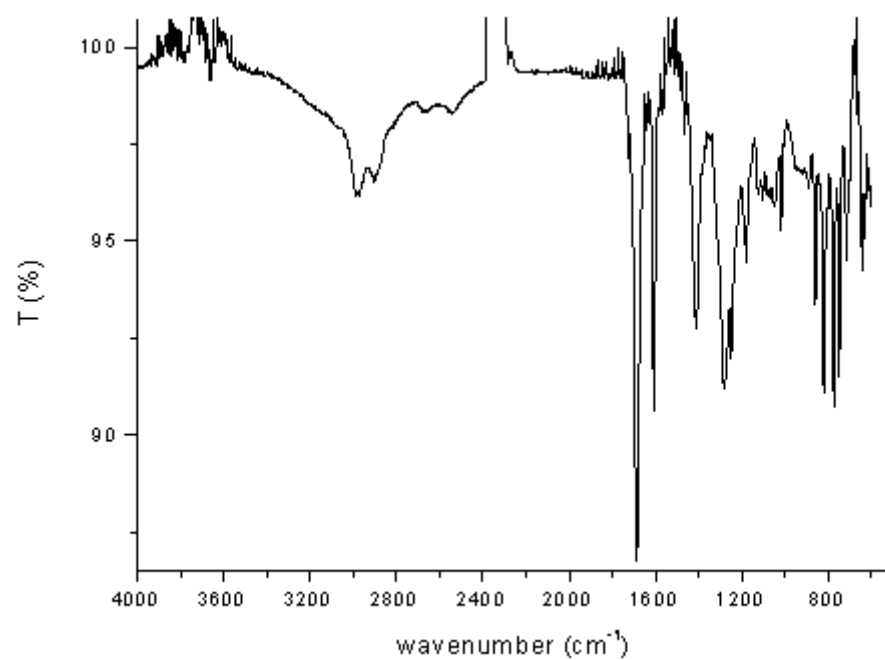


Figure S6. IR transmission spectra of **L**

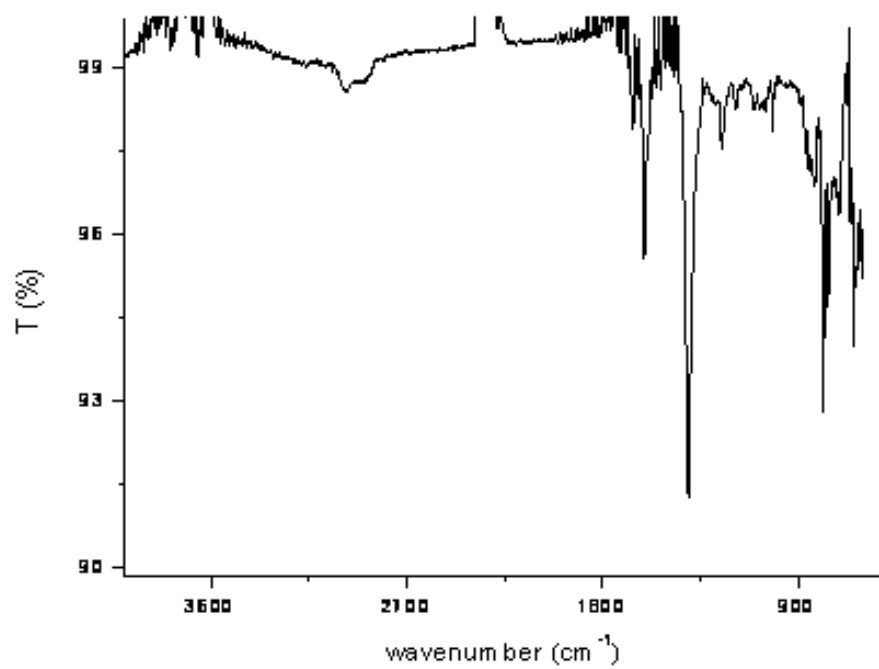


Figure S7. IR transmission spectra of **SBF-Cu**

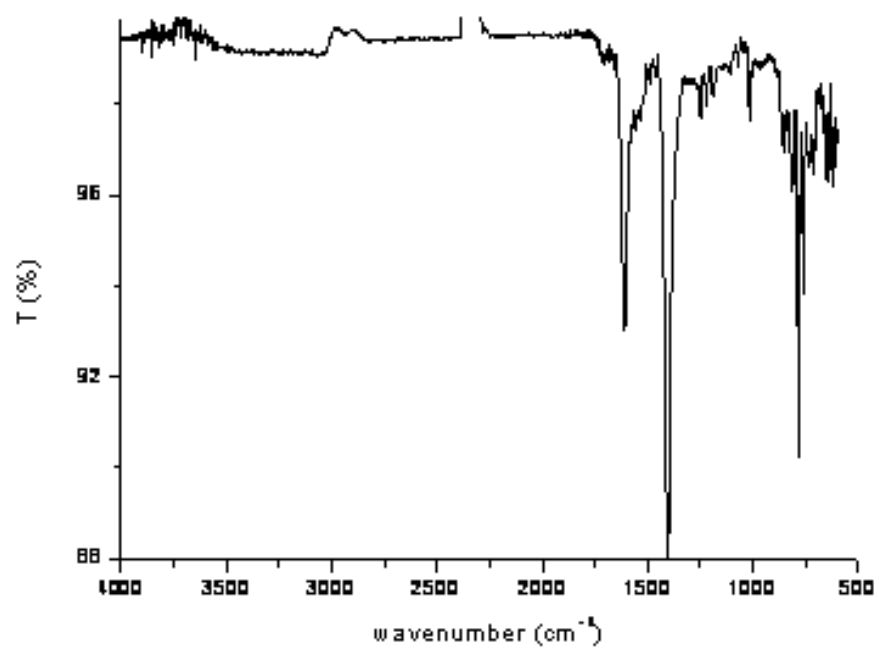


Figure S8. IR transmission spectra of **SBF-Cu\_act**

**SI-4.** UV-Vis absorption spectra of **3** and **L**

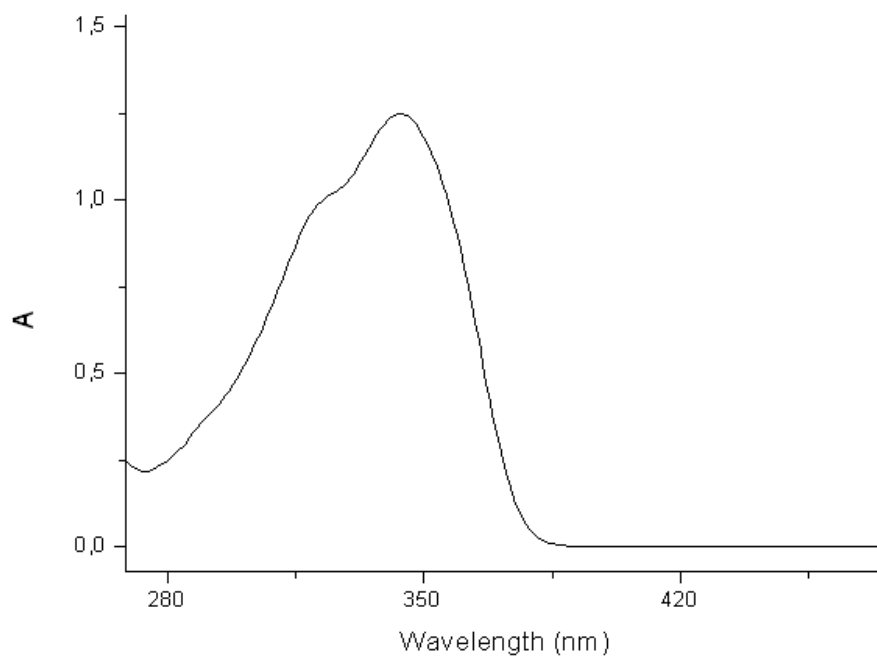


Figure S9. UV-Vis absorption spectra of **3**

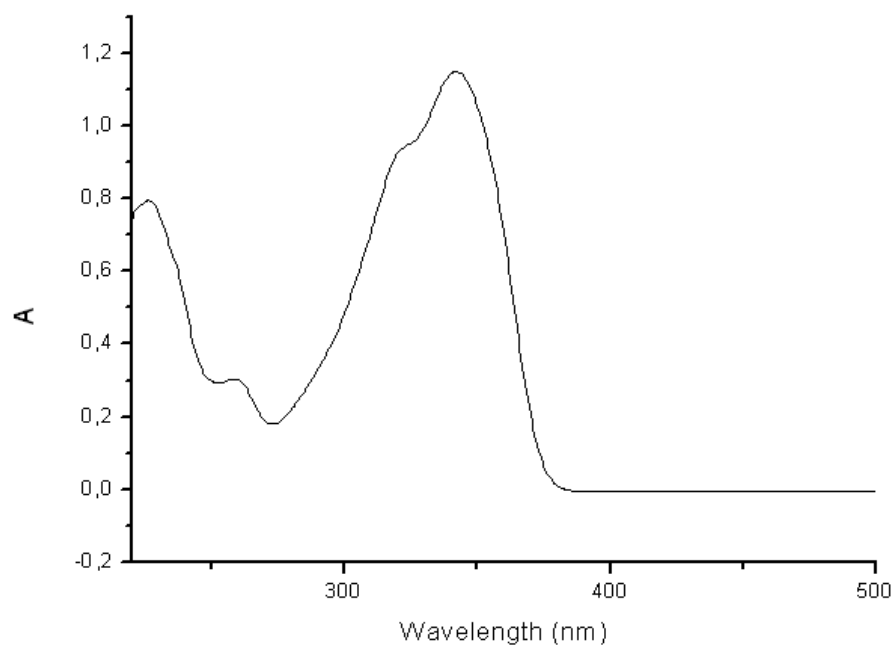


Figure S10. UV-Vis absorption spectra of **L**

**SI-5. Table S1 : Selected distances and angles within the crystal structure of SBF-Cu**

Within Copper paddle-wheel

Cu1—O2 <sup>i</sup>	1.950 (2)	O6—C27	1.246 (3)
Cu1—O6 <sup>ii</sup>	1.955 (2)	O2—C27	1.265 (4)
Cu1—O19 <sup>iii</sup>	1.961 (2)	O6—C27—O2	124.8 (3)
Cu1—O14	1.962 (2)	O19—C14	1.236 (4)
Cu1—O20	2.177 (2)	O14—C14	1.263 (4)
Cu1—Cu1 <sup>iii</sup>	2.6249 (10)	O19—C14—O14	124.7 (3)
O2 <sup>i</sup> —Cu1—O6 <sup>ii</sup>	168.23 (9)	O19 <sup>iii</sup> —Cu1—O14	167.93 (10)
O2 <sup>i</sup> —Cu1—O19 <sup>iii</sup>	89.29 (11)	O2 <sup>i</sup> —Cu1—O20	98.82 (9)
O6 <sup>ii</sup> —Cu1—O19 <sup>iii</sup>	88.41 (11)	O6 <sup>ii</sup> —Cu1—O20	92.84 (9)
O2 <sup>i</sup> —Cu1—O14	89.06 (11)	O19 <sup>iii</sup> —Cu1—O20	93.75 (10)
O6 <sup>ii</sup> —Cu1—O14	90.78 (11)	O14—Cu1—O20	98.32 (11)

Hydrogen-bond geometry (Å, °)

<i>D—H</i> ⋯ <i>A</i>	<i>D—H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D—H</i> ⋯ <i>A</i>
C23—H23⋯O6	1.10	2.49	2.796 (4)	94

<i>Metal—D</i> ⋯ <i>A</i>	<i>Metal—D</i>	<i>D</i> ⋯ <i>A</i>	<i>Meta —D</i> ⋯ <i>A</i>
Cu1—O20—Hw⋯O19 <sup>v</sup>	2.177(2)	3.243 (3)	141.58 (11)
Cu1—O20—Hw⋯O6 <sup>iv</sup>	2.177(2)	3.321 (3)	108.17 (10)

Symmetry codes: (i)  $x, y-1, -z-1/2$ ; (ii)  $x-1, -y+2, z+1/2$ ; (iii)  $-x-1, -y+1, -z$ ; (iv)  $-x, -y+2, -z$ ; (v)  $x, -y+1, z+1/2$ .

**SI-6.** Useful figures for evaluation of  $\pi$ - $\pi$  interactions between the layers of **SBF-Cu**

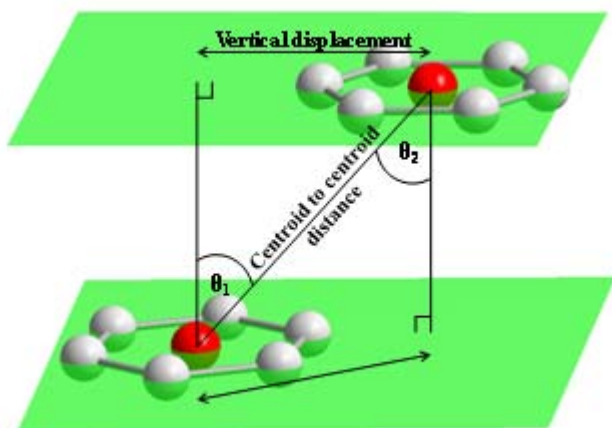


Figure S11. Parameters used for evaluation of the strength of  $\pi$ - $\pi$  interactions. ( $\theta_1$ ,  $\theta_2$ : slippage angles)

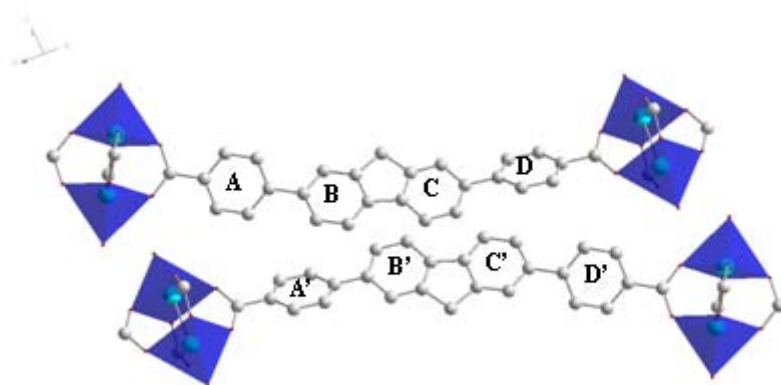


Figure S12. Representation of the closest aryl-fluorene-aryl groups from two layers of SBF-Cu.

**SI-7.** **SBF-Cu\_act** remains crystalline after gas sorption measurements.

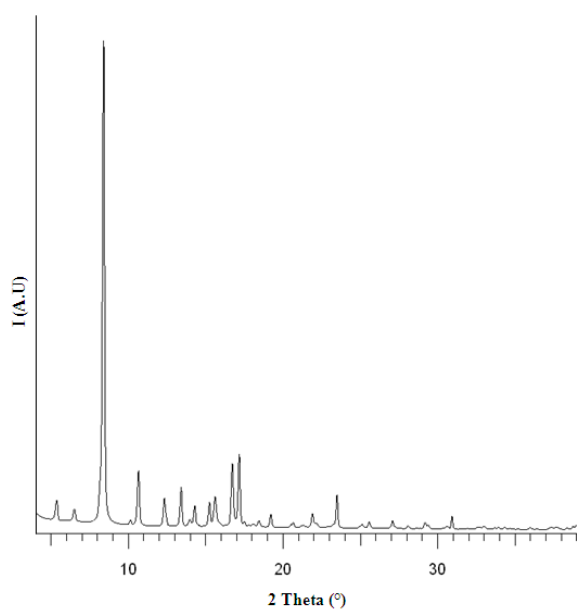


Figure S13. X-ray Powder diffraction pattern of SBF-Cu\_act after gas sorption measurements.



**SI-8.** *Asymmetric unit of the crystal structure of SBF-Cu.*

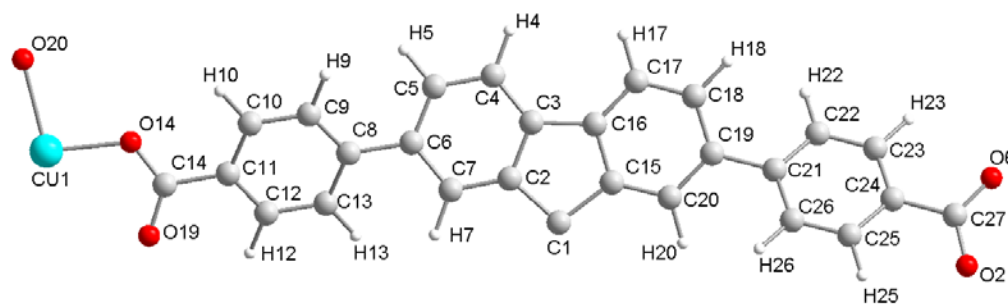


Figure S14. Representation of the asymmetric unit of the crystal structure of SBF-Cu and its atoms labels.

**SI-9.** *EDS Analysis of SBF-Cu.*

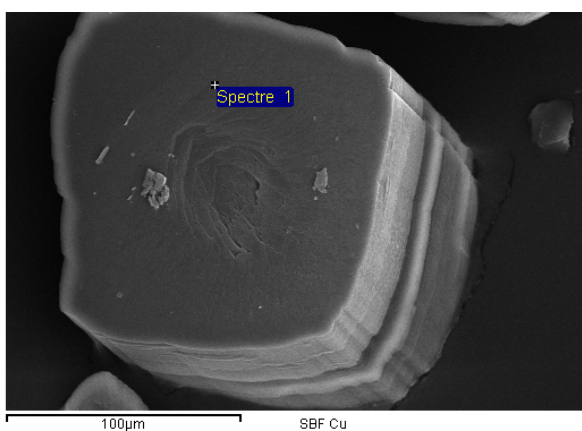


Figure S15. Scanning electron microscopy picture of a single crystal of SBF-Cu.

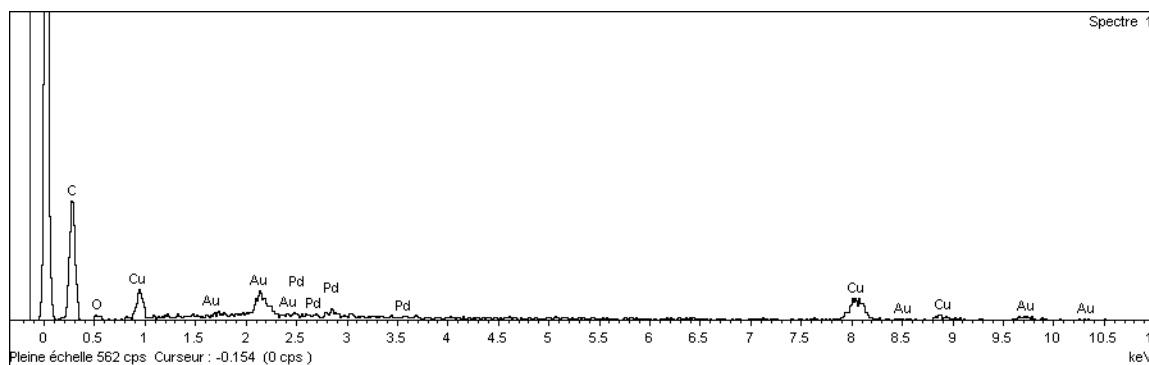


Figure S16. Energy dispersive spectrum of SBF-Cu.

Element	% Mass	% Atomic
C K	76.07	90.22
O K	6.63	5.90
Cu K	17.30	3.88

Table S2. Energy dispersive spectroscopy analysis of SBF-Cu.