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SUPPLEMENTARY MATERIAL

Engineering Isoreticular 2D Metal-Organic Frameworks with Inherent Structural Flexibility

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1. Thermogravimetric Analysis (TGA)

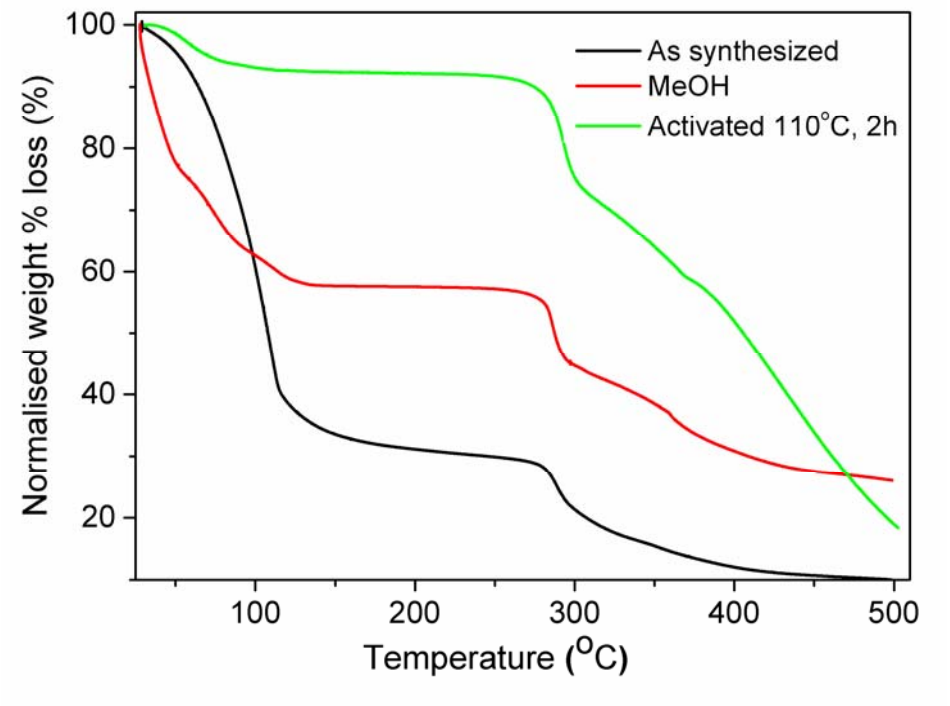

Figure SI 1. TGA traces of **CuL1Me**-*as synthesised* (black), **CuL1Me**-*MeOH exchanged* (red) and **CuL1Me**-*activated* (green).

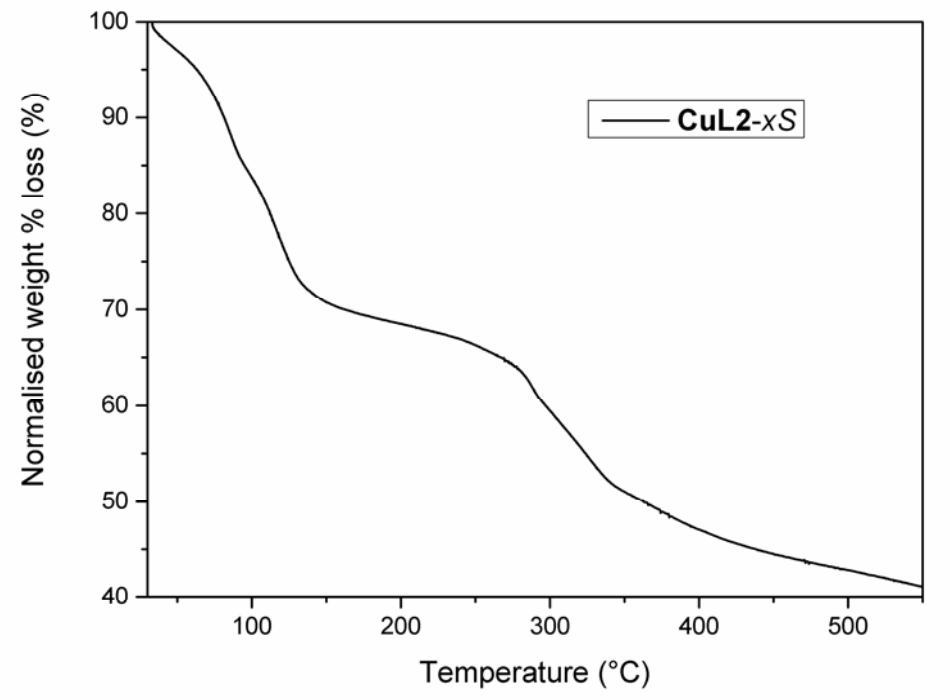

Figure SI 2. TGA trace of **CuL2**-*as synthesised*.

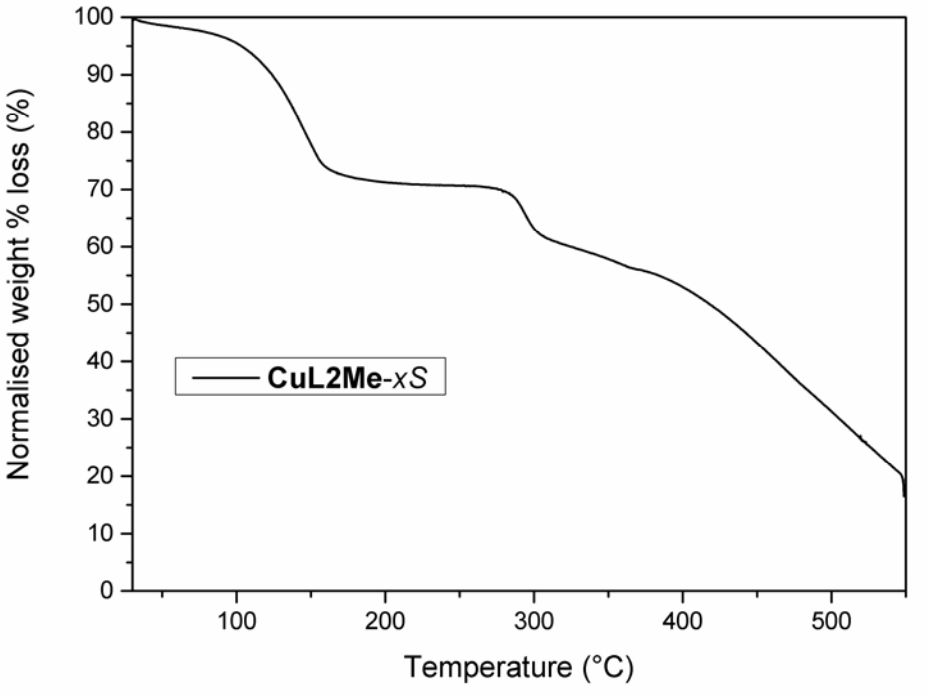

Figure SI 3. TGA trace of **CuL2Me**-*as synthesised*.

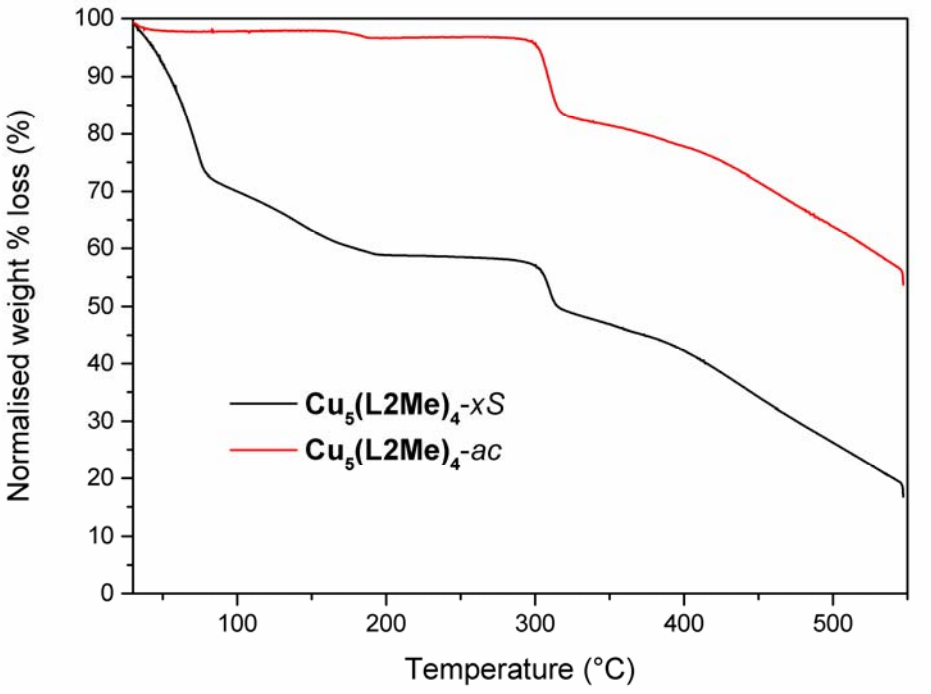

Figure SI 4. TGA traces of **Cu_5(L2Me)$_4$**-*as synthesised* (black) and **Cu_5(L2Me)$_4$**-*activated*.

2. Powder X-ray diffraction

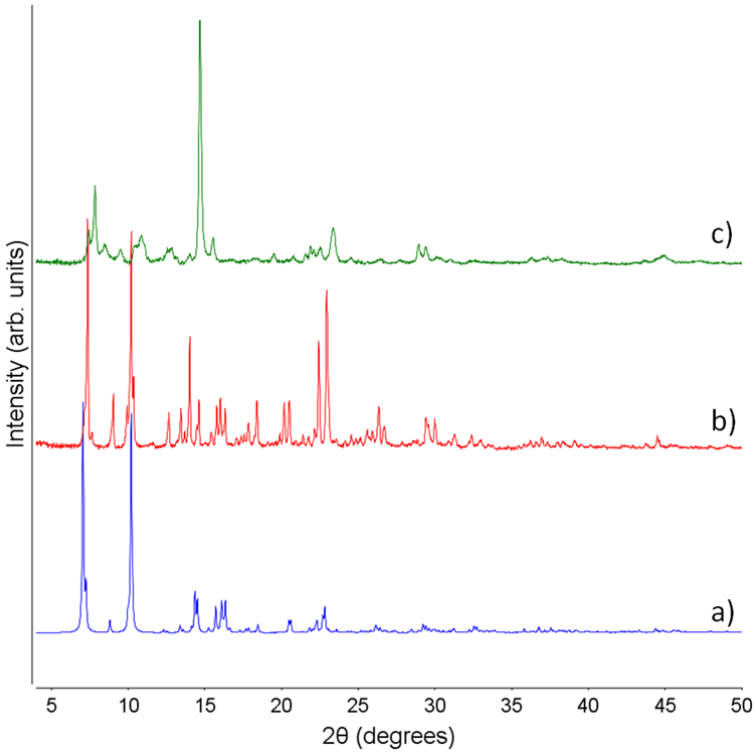

Figure SI 5. PXRD patterns of a) **CuL1Me**-*simulated*, b) **CuL1Me**-*as synthesised* and c) **CuL1Me**-*activated*. A notable structure change occurs upon activation.

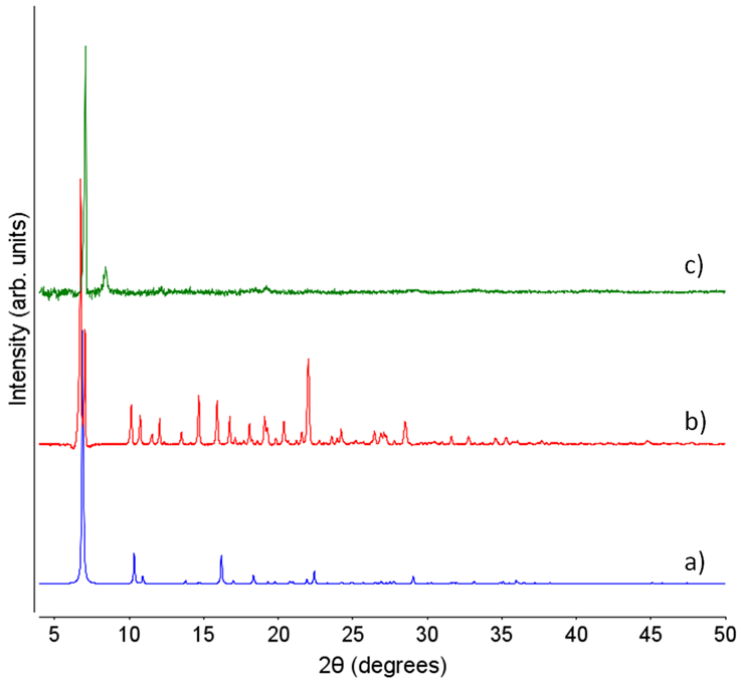

Figure SI 6. PXRD patterns of a) **CuL2Me**-*simulated*, b) **CuL2Me**-*as synthesised* and c) **CuL2Me**-*activated*.

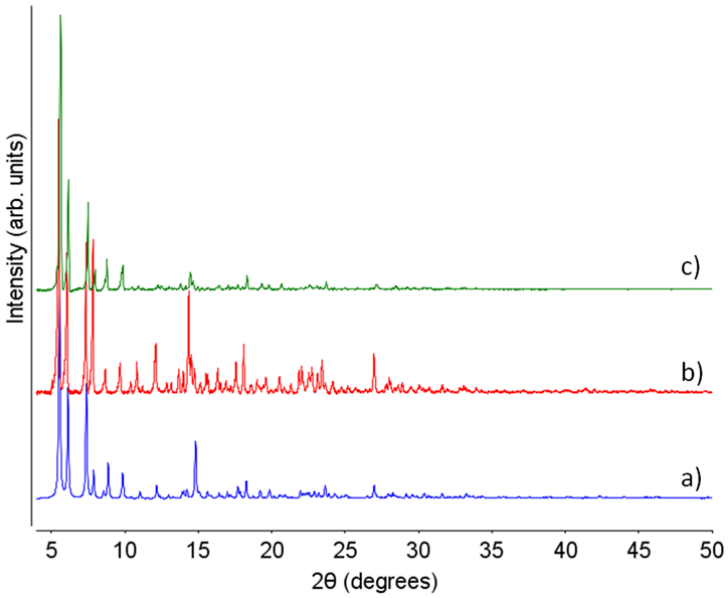

Figure SI 7. PXRD patterns of a) **$Cu_5(L2Me)_4$**-*simulated*, b) **$Cu_5(L2Me)_4$**-*as synthesised* and c) **$Cu_5(L2Me)_4$**-*activated*.

3. Variable temperature unit cell determination

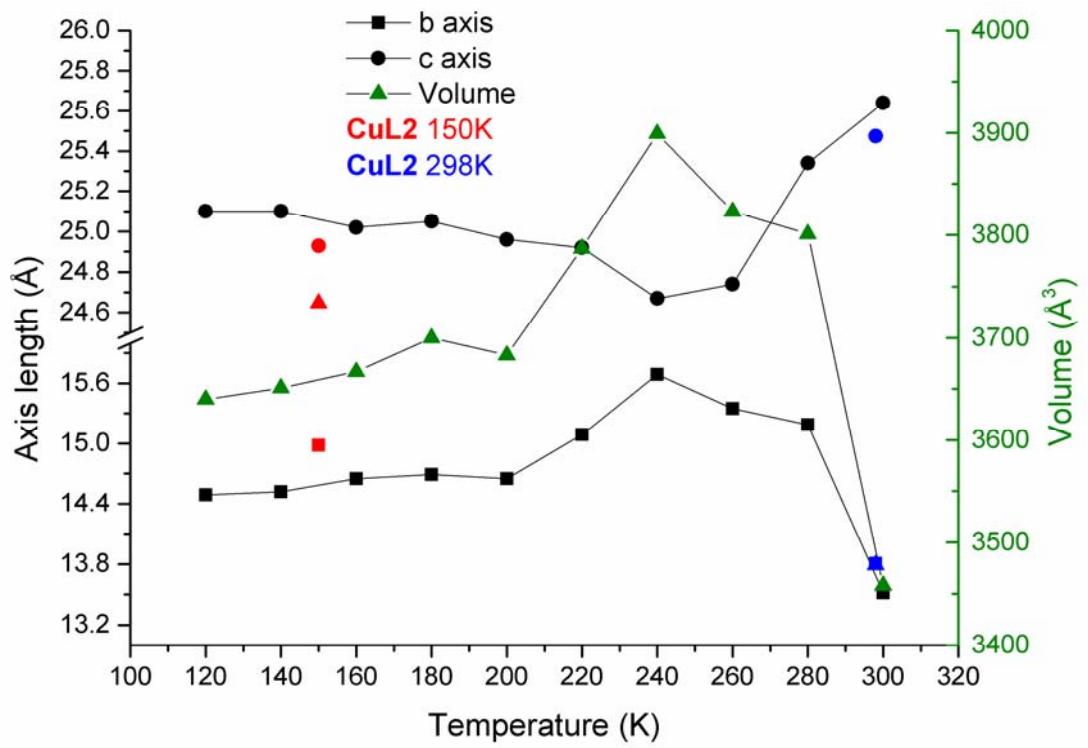

Figure SI 8. Temperature dependent changes of the unit cell axes and volume for **CuL2** determined by single crystal X-ray crystallography: black squares represent the *b* axis, black circles represent the *c* axis and green triangles represent the unit cell volume. The lines connecting data points are there to guide the eye and do not represent trend lines. The red and blue symbols (squares, circles and triangles) represent unit cell data from the X-ray crystal structures of **CuL2**collected at 150 K and 298 K respectively.

4. Gas adsorption measurements

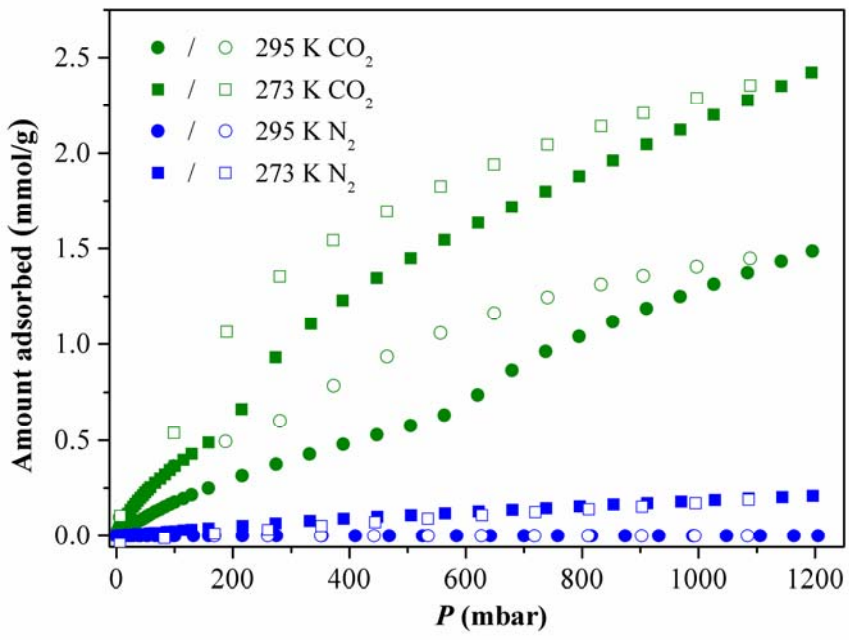

Figure SI 9. CO_2 and N_2 isotherms at 273 K and 295 K for **CuL1Me**. Closed and open symbols represent adsorption and desorption data, respectively.

Table SI1. BET parameters from the CO_2 adsorption isotherm at 195 K for **CuL1Me**.

BET Surface Area:	635.9125 ± 1.2601 m²/g
Slope:	0.006787 ± 0.000014 g/cm³ STP
Y-Intercept:	0.000058 ± 0.000001 g/cm³ STP
C:	117.401524
Qm:	146.0793 cm³/g STP
Correlation Coefficient:	0.9999821
Molecular Cross-Sectional Area:	0.1620 nm²

Table SI2. Langmuir parameters from the CO_2 adsorption isotherm at 195 K for **CuL1Me**.

Langmuir Surface Area:	732.8885 ± 11.4020 m²/g
Slope:	0.005940 ± 0.000092 g/cm³ STP
Y-Intercept:	0.077842 ± 0.005675 g/cm³ STP
b:	0.076305 1/mbar
Qm:	168.3563 cm³/g STP
Correlation Coefficient:	0.995672
Molecular Cross-Sectional Area:	0.1620 nm²

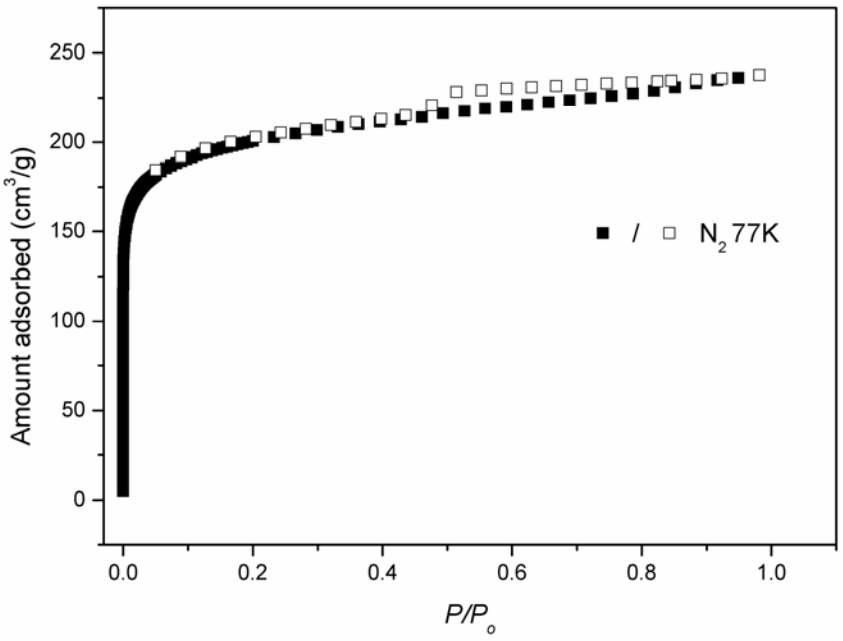

Figure SI 10. N_2 isotherm at 77K for **Cu_5(L2Me)$_4$**. Closed and open symbols represent adsorption and desorption data, respectively.

Table SI3. BET parameters from the N_2 adsorption isotherm at 77 K for **Cu_5(L2Me)$_4$**.

BET Surface Area:	759.9511 ± 2.2199 m²/g
Slope:	0.005724 ± 0.000017 g/cm³ STP
Y-Intercept:	0.000005 ± 0.000000 g/cm³ STP
C:	1206.329426
Qm:	174.5730 cm³/g STP
Correlation Coefficient:	0.9999402
Molecular Cross-Sectional Area:	0.1620 nm²

5. Accessible pore surface in $Cu_5(L2Me)_4$

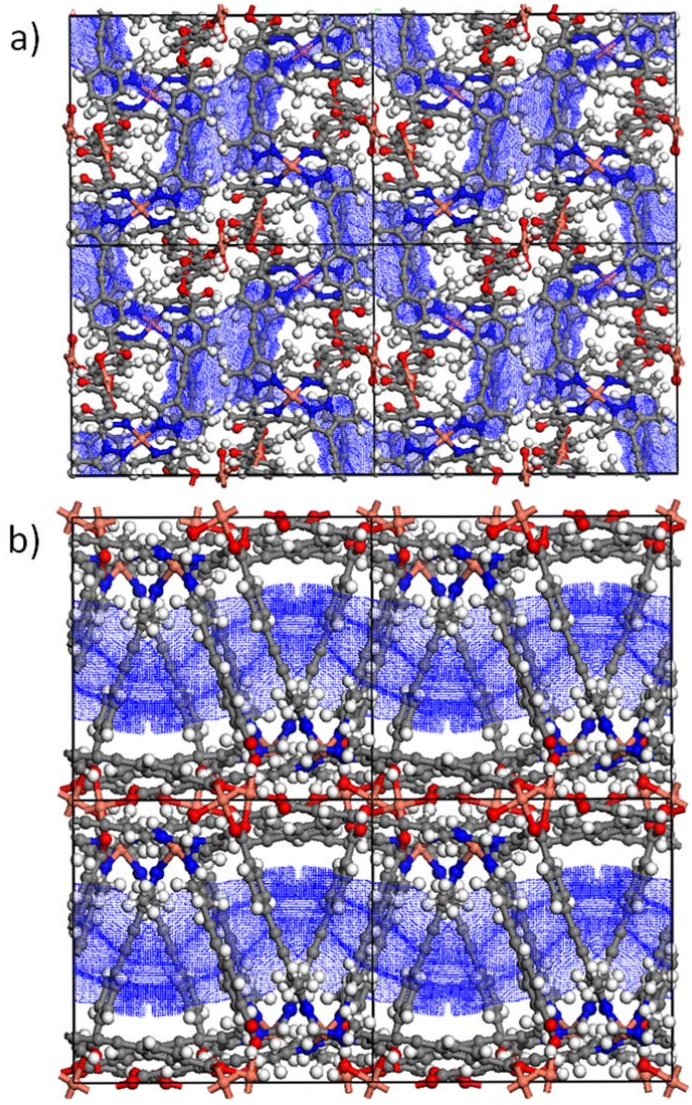

Figure SI 11. Representation of the X-ray crystal structure of **$Cu_5(L2Me)_4$** showing the solvent accessible pore surface along a) the a axis and b) the c axis.