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Supporting information for article:

A double stranded metal-organic assembly accommodating pair of water trimers in the host cavity and catalyses Glaser coupling

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Table S1 Selected torsion/dihedral angles (°) in **1**

O(1L)-C(7L)-C(9L)-C(10L)	-69.6(3)
O(2L)-C(17L)-C(19L)-C(20L)	65.9(3)
O(3L)-C(27L)-C(29L)-C(30L)	46.3(3)
C(6L)-N(1L)-C(7L)-O(1L)	71.88*
C(16L)-N(3L)-C(17L)-O(2L)	67.26*
C(26L)-N(5L)-C(27L)-O(3L)	48.00*

*Angles made by l.s. planes defined by the four atoms, with the l.s. plane of central benzene ring defined by C(9L)-C(10L)-C(19L)-C(20L)-C(29L)-C(30L), calculated using Diamond 3.0

Table S2 C-H... π interactions in **1**

No	C-H	Cg	Distance (Å)		Angle (°)
			H...C	C...Cg	
1	C12L-H12L	Cg3*	2.62	3.5618	170
2	C21L-H21L	Cg5 [#]	2.71	3.6433	166
3	C28L-H28A	Cg4 [§]	2.58	3.5331	164

Cg3 = N6L-C21L-C22L-C23L-C24L-C25L; Cg4 = C2-C3-C4-C5-C7-C8; Cg5 = C9-C10-C19-C20-C29-C30

* $\frac{1}{2}-x, -y, -\frac{1}{2}+z$, # $-\frac{1}{4}+x, \frac{1}{4}-y, -\frac{1}{4}+z$, § $\frac{3}{4}-x, \frac{1}{4}+y, \frac{3}{4}+z$

S1. Characterisation data for 1

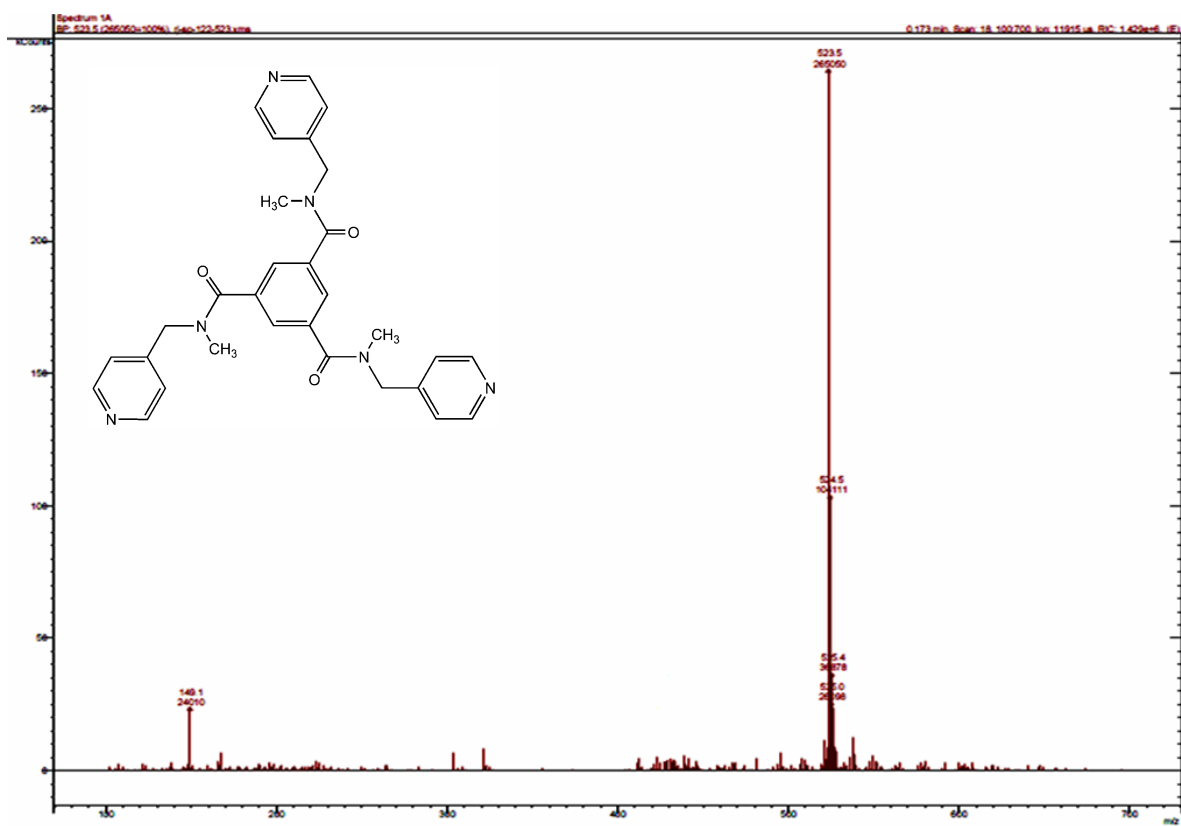


Figure S1 ESI-MS of the compound 1a

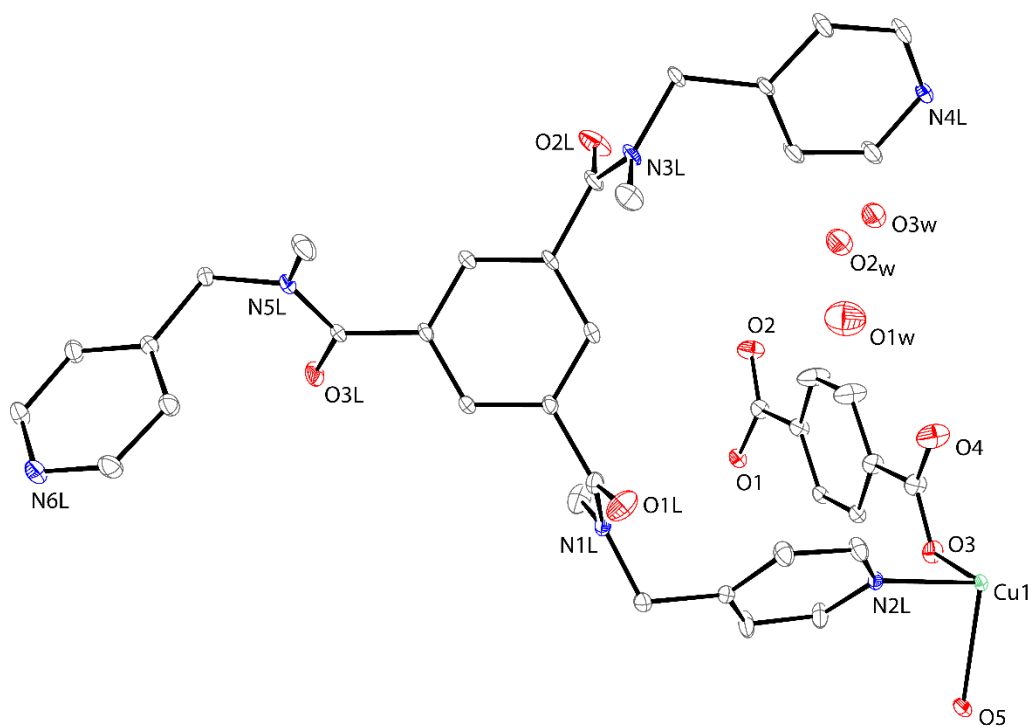
S2. Structural characterisation data and short contact interactions for 1

Figure S2 ORTEP diagram of an asymmetric unit of **1** with three H₂O molecules (H atoms are omitted for clarity).

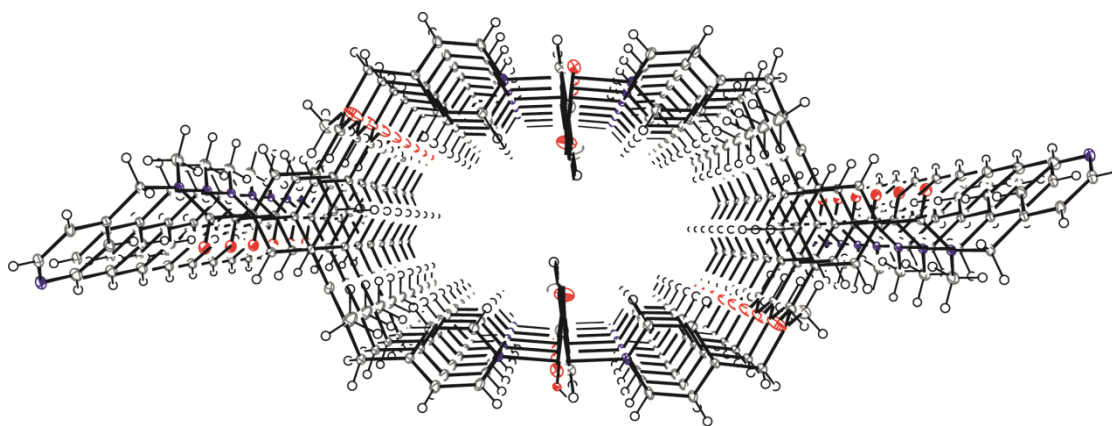


Figure S3 A perspective view of compound **1** (devoid of water cluster), showing an array of voids that accommodate acyclic water trimer pairs

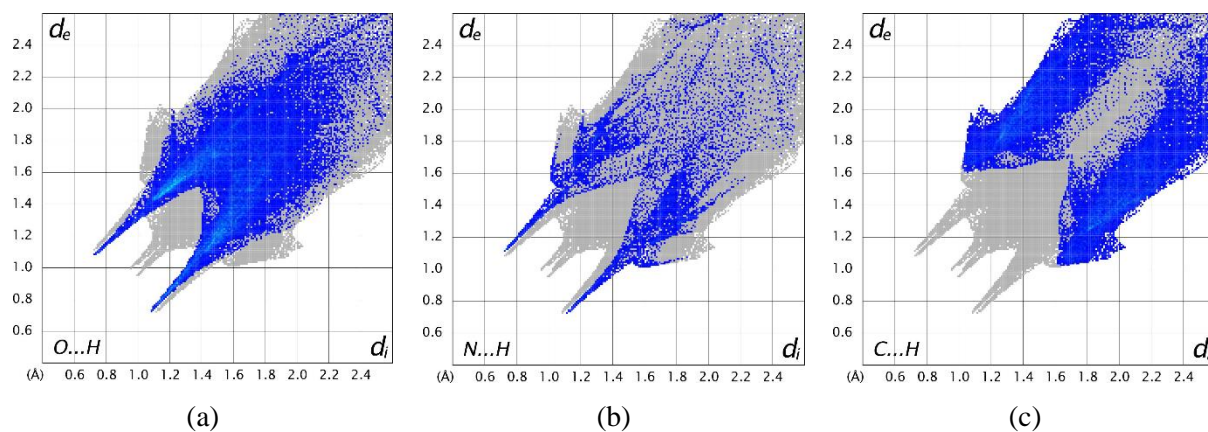


Figure S4 Fingerprint plots of (a) O-H...O, (b) N...H-O and (c) C-H...C interactions in **1**

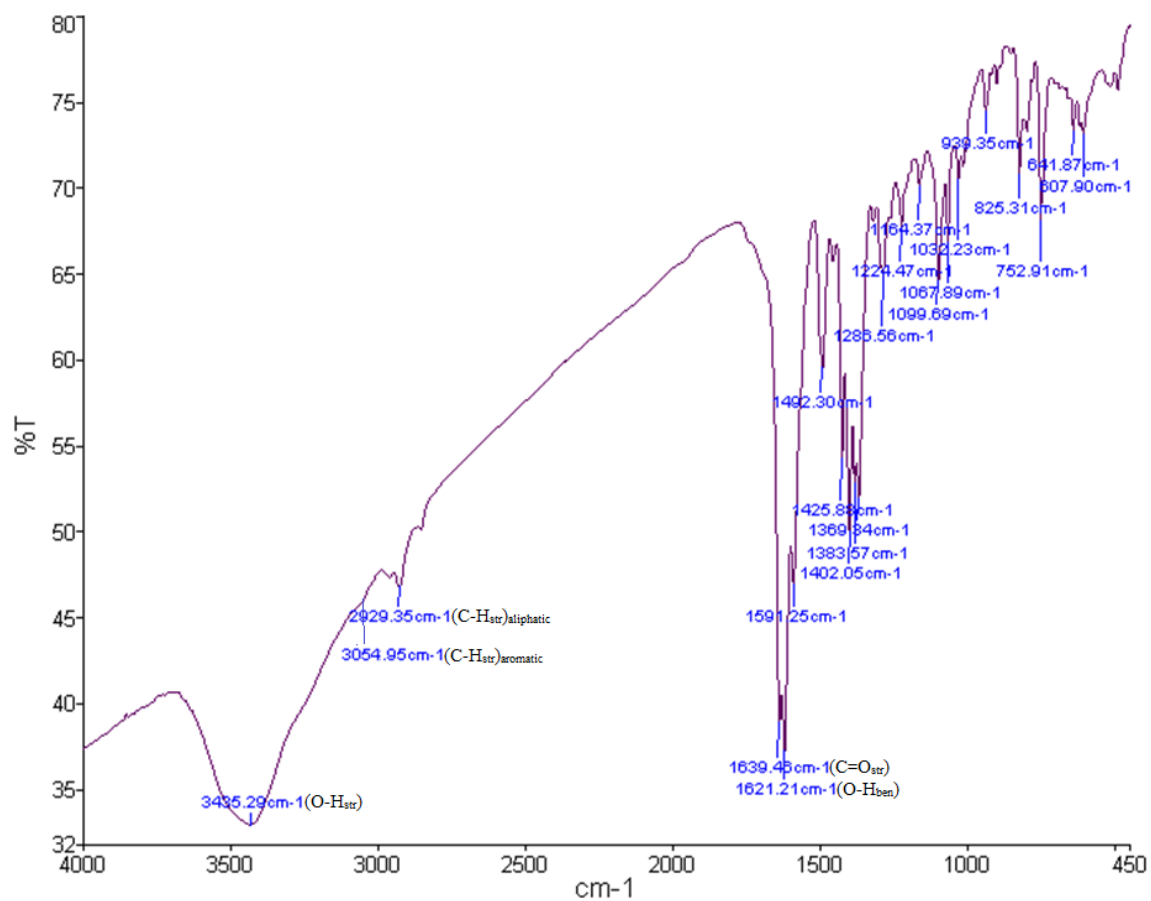


Figure S5 IR spectrum of the compound **1**.

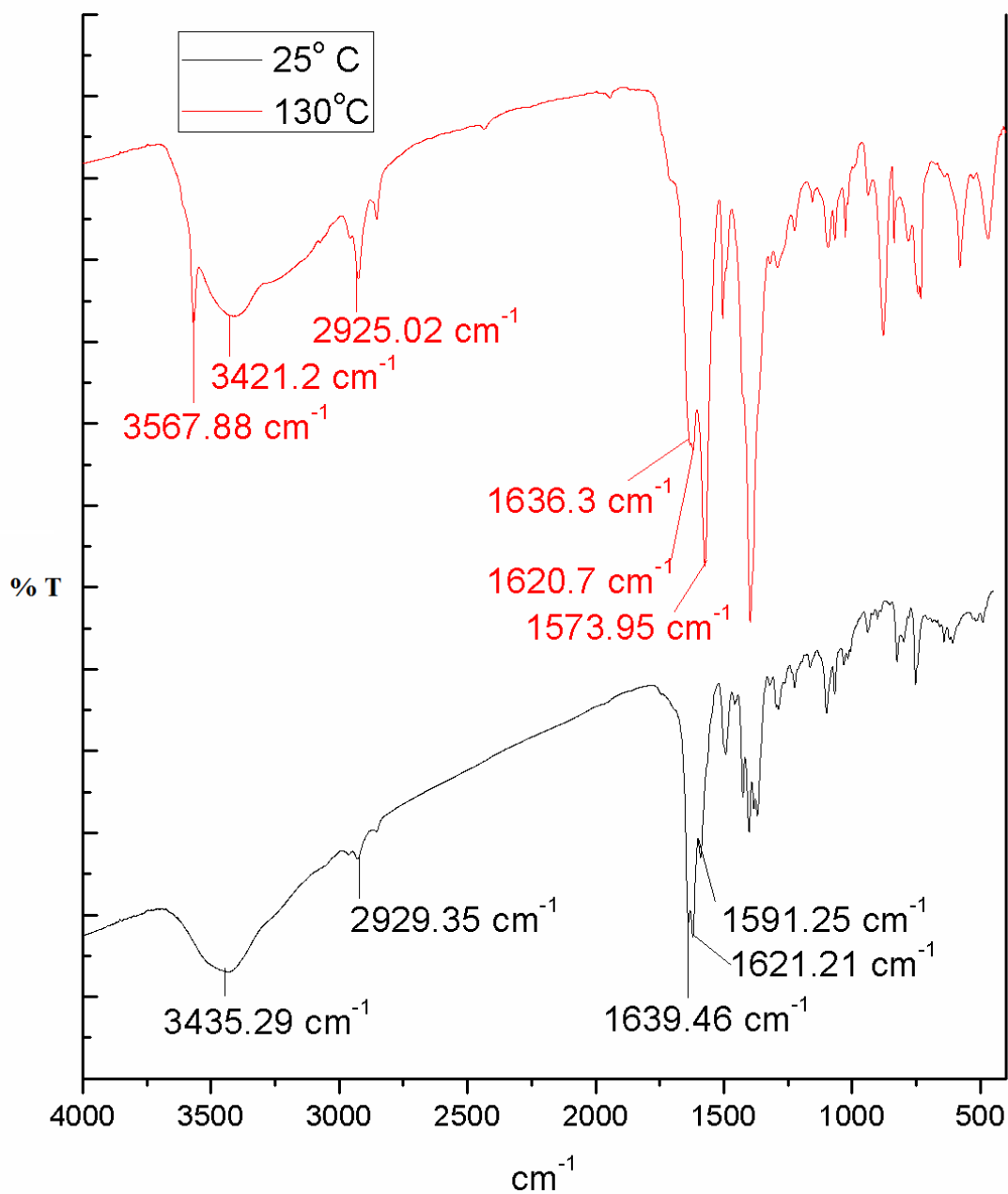


Figure S6 Comparison of the IR spectrum (KBr disc) of compound **1** as synthesized at 25°C and after heating to 130°C

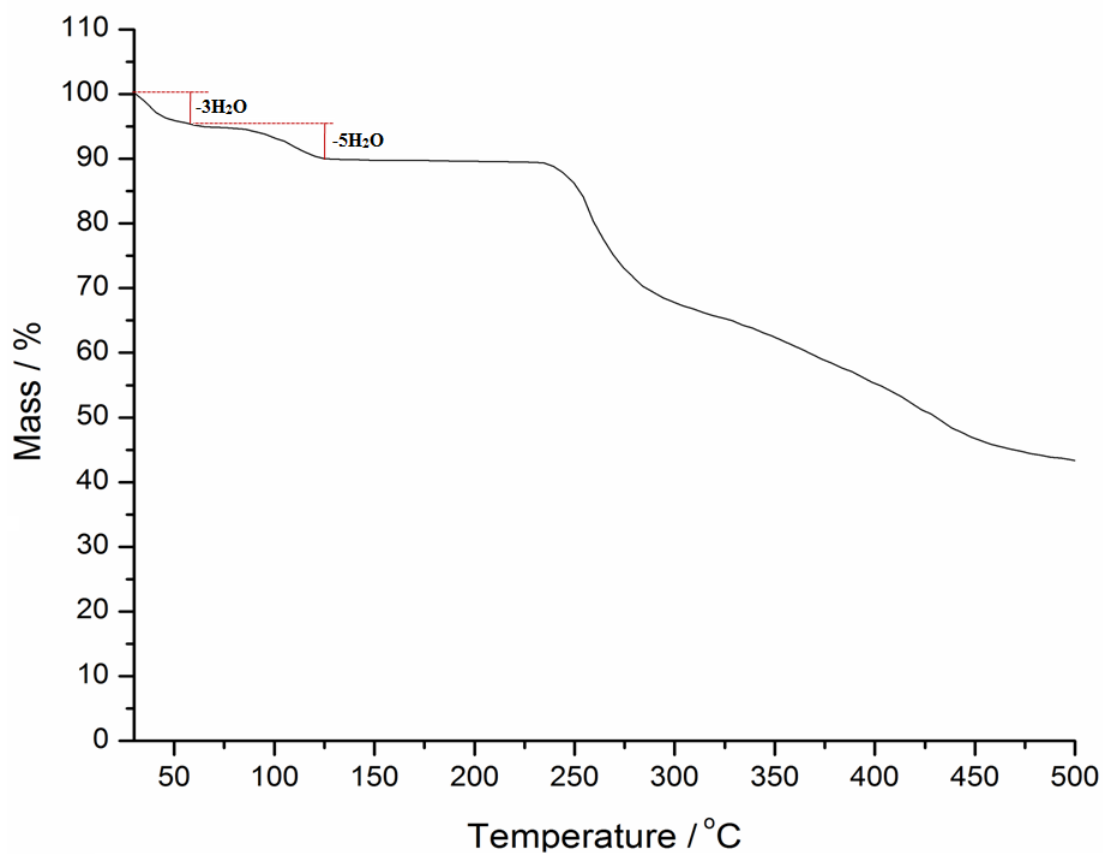


Figure S7 TGA thermogram of the compound **1**.

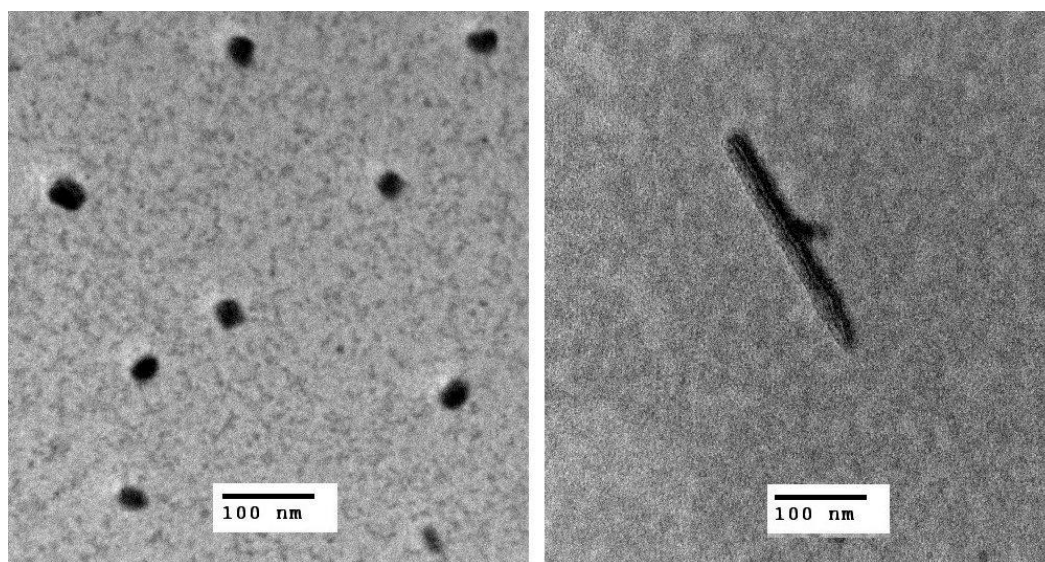


Figure S8 TEM image of compound **1**

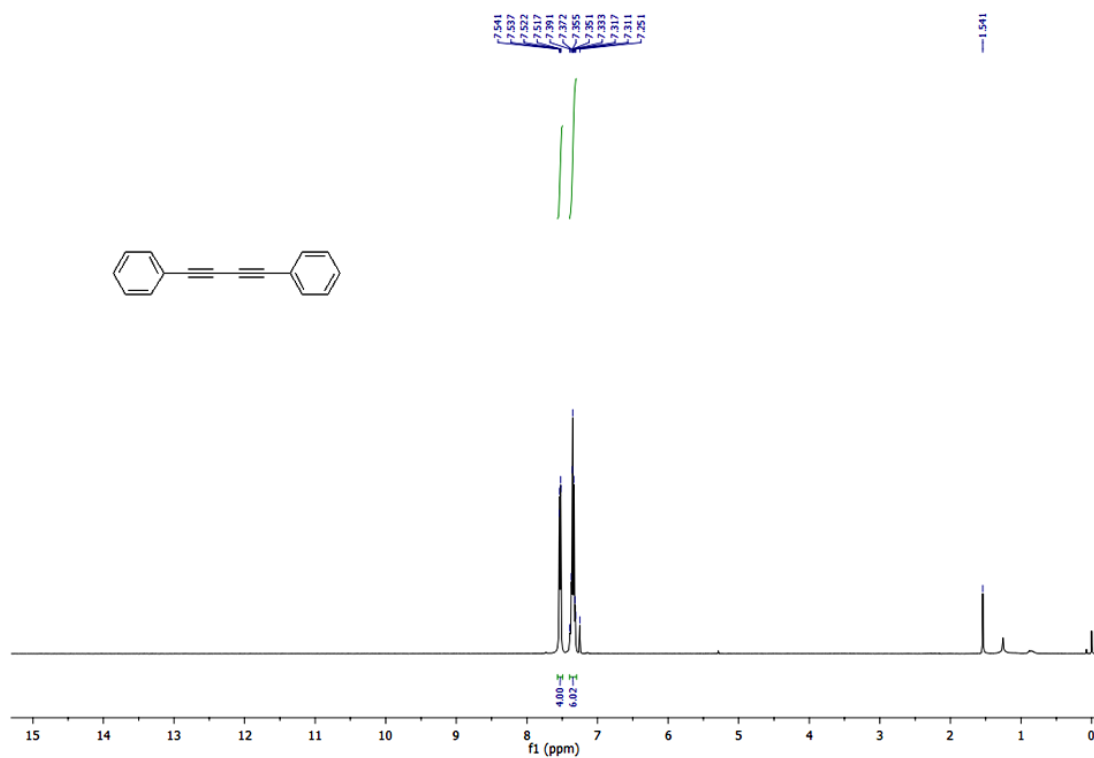


Figure S9 ¹H NMR spectrum of the product from Glaser coupling catalyzed by **1**.

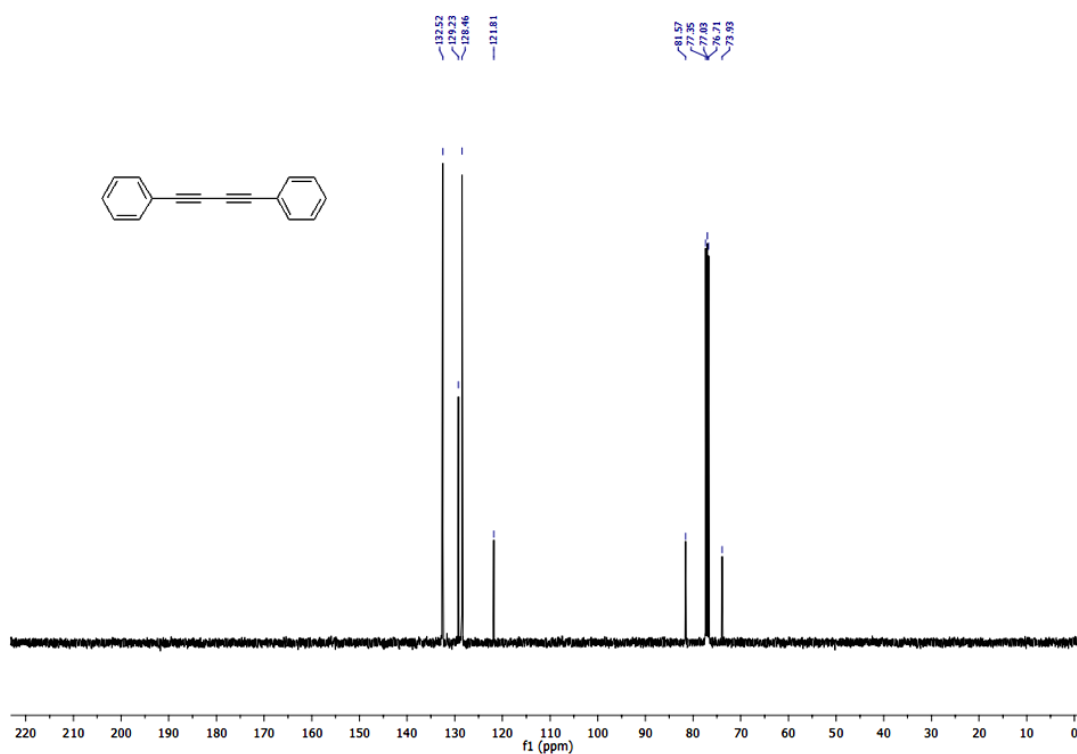


Figure S10 ¹³C NMR spectrum of the product from Glaser coupling catalyzed by **1**.

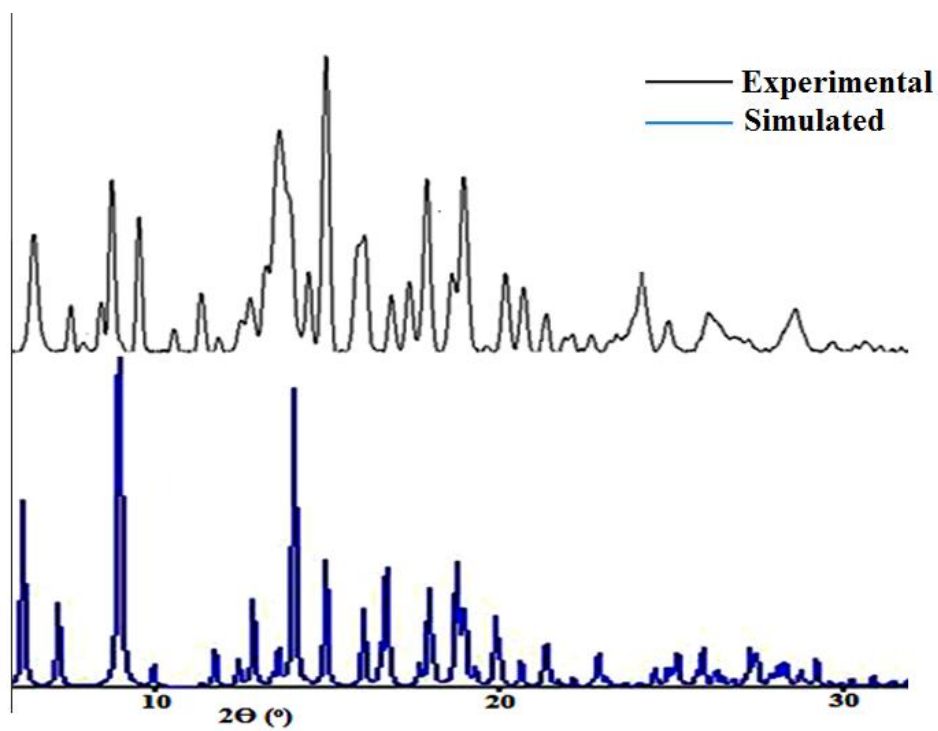


Figure S11 The experimental and simulated X-ray Powder Diffraction pattern of compound **1**