



STRUCTURAL
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Supporting information for article:

Honeycomb molecular network based upon a hydrate of 4,6-dichlororesorcinol and the photoproduct *rtct*-tetrakis(pyridin-4-yl)cyclobutane

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Supporting information

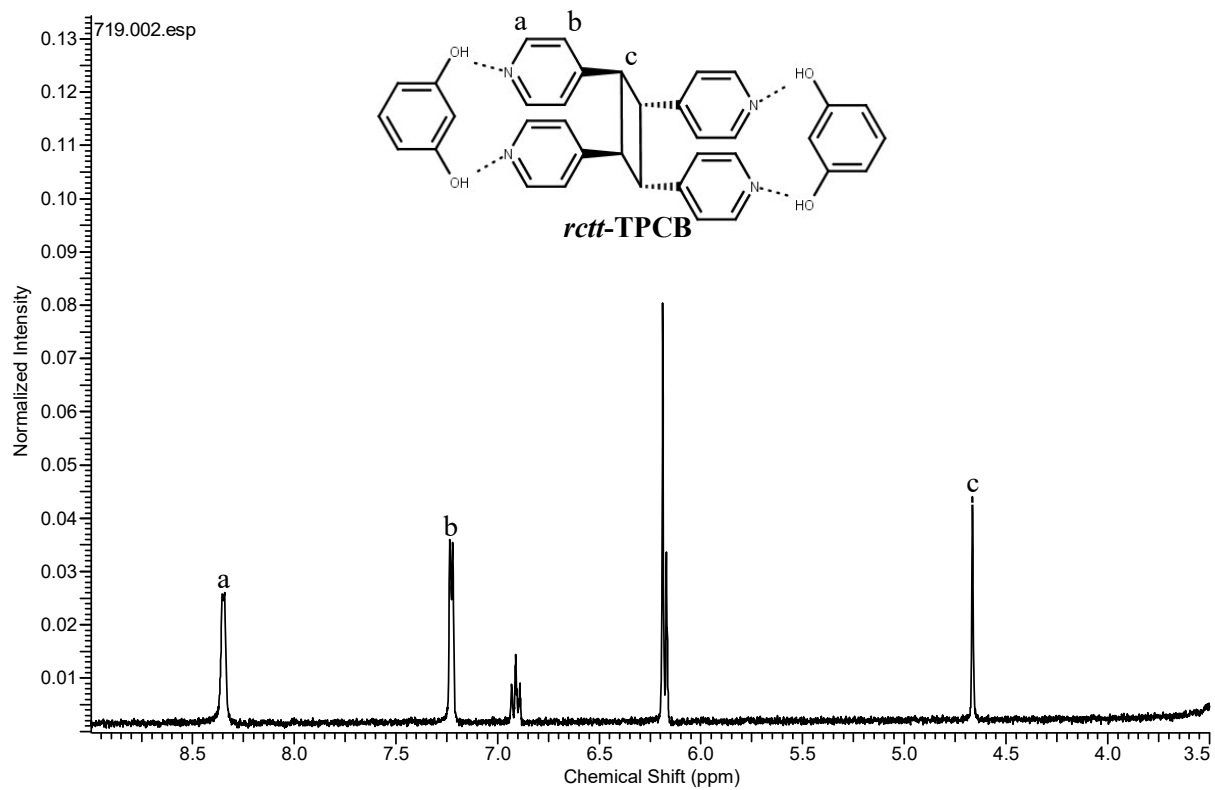


Figure S1: ^1H NMR spectrum of $2(\text{res})\cdot(\text{rctt-TPCB})$ after a quantitative [2+2] cycloaddition reaction (400 MHz, $\text{DMSO-}d_6$).

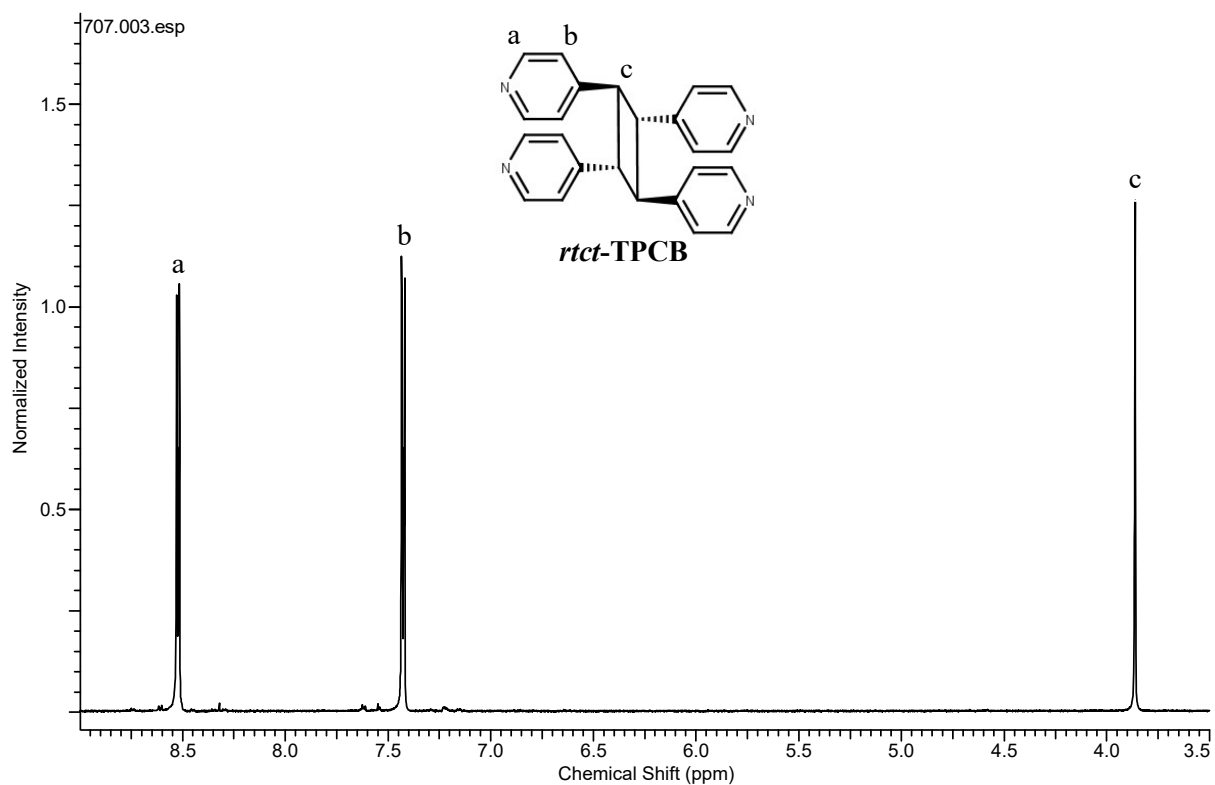


Figure S2: ^1H NMR spectrum of *rtct*-TPCB (400 MHz, DMSO- d_6).**Topology Output**

A net simplification of **(4,6-diCl res)•(*rtct*-TPCB)•(H₂O)** was performed using ToposPro software. The Auto CN and ADS commands upon choosing both the *rtct*-TPCB and water as nodes provided a simplified hcb net with a [6.6.6] topology.

Structure consists of molecules (ZA1).

Structure consists of molecules (ZB1).

Topology for ZD1

Atom ZD1 links by bridge ligands and has

Common vertex with	R(A-A)	f	Total SA
ZE 1 -0.1962 0.3751 0.2958 (-1 0 0)	7.774A	1	34.92
ZE 1 -0.1962 1.1249 0.7958 (-1 1 0)	7.906A	1	33.31
ZE 1 0.8038 0.3751 0.2958 (0 0 0)	12.929A	1	31.78

Topology for ZE1

Atom ZE1 links by bridge ligands and has

Common vertex with	R(A-A)	f	Total SA
ZD 1 1.1238 0.8686 0.5593 (1 0 0)	7.774A	1	34.58
ZD 1 1.1238 0.6314 0.0593 (1 1 -1)	7.906A	1	32.98
ZD 1 0.1238 0.8686 0.5593 (0 0 0)	12.929A	1	32.44

Structure consists of layers (0 1 0) with ZEZD

Num. groups=2; Thickness=9.14; Min.Distance=4.495

ZD1 Point symbol:{6³}

Extended point symbol:[6.6.6]

Point symbol for net: {6³}

3-c net; uninodal net

Topological type: hcb (topos&RCSR.ttd) {6³} - VS [6.6.6]