Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information for

Metal-organic polyhedron from a flexible tetrakis(thiobenzyl-carboxylate)-Tetrathiafulvalene

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SUMMARY

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Figure S3. ^{1}H NMR (300 MHz, DMSO-d_6) spectra of **L**.

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Figure S7. Mass spectra of **L**

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X-Ray structure determinations

Details about data collection and solution refinement are given in Table S1. Data collections were performed on an Agilent SuperNova diffractometer equipped with an Atlas CCD detector and micro-focus Cu-K_α radiation (λ = 1.54184 Å). The structures were solved by intrinsic phasing and refined on F^2 by full matrix least-squares techniques with SHELX programs (SHELXT 2018/2 and SHELXL 2018/3)[1–3] using the ShelXle and the Olex2 graphical user interfaces.[4,5] All non-H atoms were refined anisotropically and absorption was corrected by multiscan empirical absorption using spherical harmonics, or by numerical absorption correction based on gaussian integration over a multifaceted crystal model with CrysAlisPro program. The H atoms were placed at calculated positions and refined using a riding model. Crystallographic data for the three structures have been deposited at the Cambridge Crystallographic Data Centre, deposition numbers CCDC 2310795 for **L**, 2310797 for **Cu_8L_4-(DMAc)**, and 2310796 for **Cu_8L_4-(DMF)**. These data can be obtained free of charge from CCDC, 12 Union road, Cambridge CB2 1EZ, UK (e-mail: deposit@ccdc.cam.ac.uk or http://www.ccdc.cam.ac.uk).

PXRD measurements

Powder X-Ray diffraction (PXRD) measurements were performed on a D8 Bruker diffractometer (CuKα, λ = 1.5418 Å) equipped with a linear Vantec super speed detector.

	L	Cu_8L_4-(DMAc)	Cu_8L_4-(DMF)
Formula sum	$C_{42}H_{40}O_{10}S_{10}$	$C_{193.92}H_{194.32}Cu_8N_{10.48}O_{44.48}S_{32}$	$C_{155.90}H_{101.10}Cu_8N_{1.30}O_{41.30}S_{32}$
Formula weight	1025.34	4917.59	4187.51
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/c$	P-1	$P2_1/m$
a/Å	21.7980(12)	22.1127(6)	19.081(3)
b/Å	6.3399(5)	23.7586(6)	31.525(6)
c/Å	16.8128(10)	23.8500(5)	20.060(2)
α/°	90	95.728(2)	90
β/°	90.723(6)	94.436(2)	104.324(15)
γ/°	90	102.342(2)	90
V/Å^3	2323.3(3)	12116.4(5)	11692(3)
Z	2	2	2
D_c/g cm^{-3}	1.466	1.348	1.189
T/K	250	200	180
μ/mm^{-1}	4.867	3.891	3.929
Reflections collected	4439	25321	4566
Independent reflection	3228	16983	3178
final $R_1{}^a$, $wR_2{}^b$ [$I > 2\sigma(I)$]	0.0582, 0.1550	0.1013, 0.2782	0.1460/0.3817
$R_1{}^a$,$wR_2{}^b$ (all data)	0.0790, 0.1759	0.1269, 0.3175	0.1717/0.4082
goodness-of-fit on F^2	1.029	1.069	1.395
$\Delta\rho_{min}/\Delta\rho_{max}$ (e Å^{-3})	-0.280, 0.435	-1.058, 1.198	-0.515, 0.865
Completeness (%)	99.5	99.8	98.7
CCDC number	2310795	2310797	2310796

[a] $R_1 = \sum||F_o|-|F_c||/\sum|F_o|$. [b] $wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$; $w = 1/[\sigma^2(F_0^2)+(aP)^2+bP]$ where $P= [max(F_0^2, 0) + 2F_c^2]/3$.

Table S1 : Crystallographic data, details of data collection and structure refinement parameters.

L								
C10	C10	1.338(5)	C2A	C7A	1.37(3)	O5A	S5A	1.498(7)
C11	C9	1.345(5)	C2A	C3A	1.38(2)	S1	C9	1.744(4)
C13	C14	1.375(5)	C3A	C4A	1.35(2)	S1	C8	1.835(5)
C13	C18	1.389(6)	C4A	C5A	1.42(4)	S2	C9	1.756(4)
C13	C12	1.509(5)	C5A	C6A	1.38(3)	S2	C10	1.761(4)
C15	C14	1.382(5)	C6A	C7A	1.33(2)	S3	C11	1.757(4)
C16	C17	1.375(5)	C8	C5A	1.54(2)	S3	C10	1.758(3)
C16	C15	1.380(5)	O1A	C1A	1.15(2)	S4	C11	1.759(3)
C16	C19	1.497(5)	O2A	C1A	1.34(2)	S4	C12	1.815(4)
C17	C18	1.378(5)	O3	C19	1.194(6)	S5A	C21A	1.55(2)
C1A	C2A	1.49(2)	O4	C19	1.304(6)	S5A	C20A	1.79(1)

Table S2. Selected bond distances (Å) for compound **L.**

Cu_8L_4-(DMAc)

C10A	C11A	1.39(1)	C1C	C2C	1.47(2)	C28A	C27A	1.43(2)	C35A	C34A	1.39(2)
C10A	C13A	1.39(2)	C1D	C2D	1.50(1)	C28B	C29B	1.42(2)	C35B	C34B	1.40(2)
C10B	C9B	1.28(2)	C1I	N1I	1.44(3)	C29A	C30A	1.49(1)	C35C	C36C	1.38(1)
C10C	C9C	1.29(1)	C1M	N1M	1.45(3)	C29C	C28C	1.34(2)	C35C	C34C	1.42(2)
C11A	C12A	1.38(2)	C1O'	N1O'	1.30(2)	C29D	C28D	1.37(2)	C35D	C34D	1.39(2)
C11B	C12B	1.26(2)	C1O'	C4O'	1.51(4)	C2A	C3A	1.36(2)	C35D	C36D	1.40(2)
C11D	C12D	1.28(2)	C20A	C19A	1.30(2)	C2A	C7A	1.41(2)	C36A	C37A	1.39(2)
C12C	C11C	1.34(2)	C20B	C21B	1.40(2)	C2B	C3B	1.35(1)	C36B	C35B	1.35(2)
C13A	C14A	1.39(2)	C21C	C20C	1.39(1)	C2B	C7B	1.39(2)	C36B	C37B	1.42(2)
C14B	C13B	1.45(2)	C21D	C20D	1.39(2)	C2B	C1B	1.49(2)	C36C	C37C	1.36(1)
C14C	C13C	1.29(1)	C22A	C21A	1.34(2)	C2C	C7C	1.40(2)	C37B	C38B	1.33(2)
C14D	C13D	1.29(2)	C22B	C19B	1.50(2)	C2C	C3C	1.40(2)	C37D	C36D	1.40(2)
C15A	C12A	1.37(2)	C22C	C19C	1.49(1)	C2D	C3D	1.40(1)	C38A	C35A	1.50(1)
C15A	C14A	1.39(2)	C24A	C27A	1.37(2)	C2D	C7D	1.41(2)	C38B	C39B	1.41(2)
C15A	C16A	1.56(2)	C24A	C25A	1.40(2)	C2G	N1G	1.46(5)	C38C	C35C	1.45(1)
C16B	C17B	1.34(2)	C24A	C23A	1.52(2)	C2I	N1I	1.44(2)	C38D	C35D	1.50(1)
C16B	C21B	1.42(2)	C24B	C25B	1.37(2)	C2L	N1L	1.46(4)	C39B	C34B	1.38(2)
C16B	C15B	1.56(2)	C24B	C29B	1.38(2)	C2M	N1M	1.45(4)	C39B	C32B	1.52(2)
C16C	C21C	1.39(1)	C24B	C23B	1.55(2)	C2R	N1R	1.44(3)	C3A	C4A	1.44(2)
C16C	C15C	1.51(1)	C24C	C29C	1.35(2)	C30A	C28A	1.38(2)	C3B	C4B	1.39(2)
C16D	C17D	1.36(2)	C24C	C25C	1.39(2)	C30A	C26A	1.39(1)	C3C	C4C	1.43(2)
C16D	C21D	1.39(2)	C24C	C23C	1.49(2)	C30B	C27B	1.53(2)	C3E	C4E	1.49(2)
C16D	C15D	1.50(2)	C24D	C29D	1.37(2)	C30C	C27C	1.49(2)	C3F	C4F	1.55(2)
C17C	C16C	1.39(2)	C24D	C25D	1.38(2)	C32A	C33A	1.37(2)	C3G	N1G	1.32(4)
C18A	C17A	1.32(2)	C24D	C23D	1.48(2)	C32A	C37A	1.39(2)	C3G	C4G	1.49(5)
C18B	C17B	1.38(2)	C25D	C26D	1.37(2)	C32A	C31A	1.51(2)	C3H	C4H	1.52(2)
C18C	C19C	1.39(1)	C26A	C25A	1.39(2)	C32C	C37C	1.39(2)	C3I	N1I	1.31(2)
C18C	C17C	1.40(1)	C26B	C25B	1.37(2)	C32C	C33C	1.42(1)	C3I	C4I	1.50(2)
C18D	C17D	1.43(2)	C26C	C25C	1.38(2)	C32C	C31C	1.47(1)	C3J	C4J	1.49(2)
C19B	C20B	1.36(2)	C27B	C28B	1.31(2)	C32D	C37D	1.35(2)	C3L	N1L	1.32(3)
C19B	C18B	1.41(2)	C27B	C26B	1.38(2)	C32D	C33D	1.41(2)	C3L	C4L	1.49(3)
C19C	C20C	1.38(1)	C27C	C26C	1.37(2)	C32D	C31D	1.49(1)	C3M	O1M	1.21(3)
C19D	C20D	1.34(2)	C27C	C28C	1.41(2)	C33C	C34C	1.37(2)	C3M	N1M	1.32(3)
C19D	C18D	1.38(2)	C27D	C26D	1.38(2)	C34A	C33A	1.38(2)	C3M	C4M	1.48(4)
C19D	C22D	1.51(2)	C27D	C28D	1.41(2)	C34D	C33D	1.37(2)	C3P	C4P	1.53(2)
C1A	C2A	1.48(2)	C27D	C30D	1.51(2)	C35A	C36A	1.38(2)	C3Q	C4Q	1.54(3)

C3R	O1R	1.20(3)	Cu3	O6C	1.969(8)	N1F	C2F	1.47(2)	O2A	C1A	1.25(2)
C3R	N1R	1.34(3)	Cu3	O7A	1.985(8)	N1F	C1F	1.56(3)	O2B	C1B	1.27(1)
C3R	C4R	1.48(3)	Cu3	O5D	1.994(7)	N1G	C1G	1.46(4)	O2C	C38C	1.26(1)
C40B	C36B	1.51(2)	Cu3	O1P	2.13(1)	N1H	C3H	1.33(1)	O2D	C38D	1.22(1)
C4D	C3D	1.37(2)	Cu4	O5C	1.952(8)	N1H	C2H	1.44(2)	O3A	C29A	1.28(1)
C4K	C3K	1.78(3)	Cu4	O6D	1.962(6)	N1H	C1H	1.48(2)	O3B	C40B	1.25(2)
C5A	C4A	1.36(2)	Cu4	O1A	1.966(8)	N1J	C3J	1.35(2)	O3C	C22C	1.27(1)
C5A	C6A	1.37(2)	Cu4	O8A	1.967(7)	N1J	C1J	1.42(2)	O3D	C15D	1.26(1)
C5A	C8A	1.50(2)	Cu4	O1F	2.122(8)	N1J	C2J	1.46(2)	O4A	C29A	1.24(1)
C5B	C4B	1.34(2)	Cu4	Cu3	2.643(2)	N1K	C3K	1.01(4)	O4B	C40B	1.24(1)
C5B	C6B	1.42(2)	Cu5	O1D	1.928(7)	N1K	C2K	1.51(3)	O4C	C22C	1.25(1)
C5B	C8B	1.46(2)	Cu5	O5A	1.932(7)	N1K	C1K	1.77(3)	O4D	C15D	1.25(2)
C5C	C6C	1.38(2)	Cu5	O3D	1.999(8)	N1L	C1L	1.46(4)	O5A	C9A	1.25(1)
C5C	C4C	1.38(2)	Cu5	O2B	2.017(7)	N1O'	C2O'	1.45(3)	O5B	C30B	1.23(2)
C5C	C8C	1.49(2)	Cu5	O1E	2.162(8)	N1O'	C3O'	1.47(3)	O5C	C1C	1.26(1)
C5D	C6D	1.38(2)	Cu6	O1B	1.949(9)	N1P	C3P	1.32(1)	O5D	C1D	1.23(1)
C5D	C4D	1.39(2)	Cu6	O4D	1.951(9)	N1P	C1P	1.45(2)	O5O'	C1O'	1.18(2)
C5D	C8D	1.49(2)	Cu6	O2D	1.993(7)	N1P	C2P	1.46(2)	O6A	C9A	1.27(1)
C7A	C6A	1.40(2)	Cu6	O6A	2.005(7)	N1Q	C3Q	1.33(2)	O6B	C30B	1.29(2)
C7B	C6B	1.40(2)	Cu6	O2N	2.171(7)	N1Q	C2Q	1.45(2)	O6C	C1C	1.27(1)
C7C	C6C	1.38(2)	Cu6	Cu5	2.655(2)	N1Q	C1Q	1.46(2)	O6D	C1D	1.27(1)
C7D	C6D	1.33(2)	Cu7	O5B	1.91(1)	N1R	C1R	1.42(3)	O7A	C38A	1.26(1)
C9A	C10A	1.49(2)	Cu7	O8D	1.910(9)	O1A	C1A	1.28(1)	O7B	C22B	1.28(2)
C9D	C10D	1.33(2)	Cu7	O7C	1.977(8)	O1B	C1B	1.24(1)	O7C	C30C	1.20(2)
Cu1	O2C	1.942(8)	Cu7	O3B	2.00(1)	O1C	C38C	1.28(1)	O7D	C30D	1.24(2)
Cu1	O3A	1.951(7)	Cu7	O5O'	2.10(1)	O1D	C38D	1.29(1)	O8A	C38A	1.25(1)
Cu1	O4C	2.013(7)	Cu8	O7D	1.946(7)	O1E	C3E	1.21(2)	O8B	C22B	1.23(1)
Cu1	O7B	2.032(8)	Cu8	O8C	1.950(7)	O1F	C3F	1.21(2)	O8C	C30C	1.31(1)
Cu1	O1N	2.145(6)	Cu8	O4B	1.961(8)	O1G	C3G	1.22(4)	O8D	C30D	1.27(1)
Cu2	O8B	1.915(7)	Cu8	O6B	1.986(8)	O1H	C3H	1.25(1)	S1A	C18A	1.73(1)
Cu2	O3C	1.924(7)	Cu8	O1K	2.168(8)	O1I	C3I	1.20(2)	S1A	C8A	1.80(2)
Cu2	O4A	1.998(8)	Cu8	Cu7	2.636(2)	O1J	C3J	1.21(2)	S1B	C10B	1.72(1)
Cu2	O1C	2.008(7)	N1E	C3E	1.31(2)	O1K	C3K	1.19(3)	S1B	C32B	1.77(2)
Cu2	O1H	2.127(6)	N1E	C1E	1.49(2)	O1L	C3L	1.22(4)	S1C	C14C	1.75(1)
Cu2	Cu1	2.642(2)	N1E	C2E	1.54(3)	O1P	C3P	1.20(1)	S1C	C31C	1.86(1)
Cu3	O2A	1.940(8)	N1F	C3F	1.29(2)	O1Q	C3Q	1.20(2)	S1D	C13D	1.77(1)
S1D	C23D	1.82(1)	S2A	C16A	1.83(2)	S2B	C8B	1.85(1)	S2C	C23C	1.86(1)
S2A	C17A	1.79(1)	S2B	C9B	1.76(1)	S2C	C13C	1.76(1)	S2D	C14D	1.74(1)

S2D	C31D	1.81(1)	S4B	C10B	1.85(1)	S5D	C9D	1.79(1)	S7B	C15B	1.90(2)
S3A	C19A	1.77(1)	S4C	C12C	1.75(1)	S6A	C20A	1.73(1)	S7C	C9C	1.75(1)
S3A	C18A	1.80(1)	S4C	C14C	1.79(1)	S6A	C22A	1.80(1)	S7C	C8C	1.83(1)
S3B	C9B	1.77(1)	S4D	C12D	1.76(1)	S6B	C13B	1.73(2)	S7D	C10D	1.74(1)
S3B	C11B	1.81(2)	S4D	C13D	1.77(1)	S6B	C12B	1.77(2)	S7D	C22D	1.77(1)
S3C	C13C	1.77(1)	S5A	C21A	1.76(1)	S6C	C11C	1.78(1)	S8A	C22A	1.73(1)
S3C	C12C	1.77(1)	S5A	C20A	1.81(1)	S6C	C9C	1.79(1)	S8A	C23A	1.80(1)
S3D	C12D	1.78(1)	S5B	C14B	1.75(1)	S6D	C10D	1.77(1)	S8B	C14B	1.70(1)
S3D	C14D	1.79(1)	S5B	C12B	1.81(2)	S6D	C11D	1.79(1)	S8B	C23B	1.76(2)
S4A	C17A	1.71(1)	S5C	C11C	1.74(1)	S7A	C21A	1.75(1)	S8C	C10C	1.77(1)
S4A	C19A	1.79(1)	S5C	C10C	1.75(1)	S7A	C31A	1.83(1)	S8C	C15C	1.82(1)
S4B	C11B	1.77(1)	S5D	C11D	1.75(1)	S7B	C13B	1.70(1)	S8D	C9D	1.73(1)
S8D	C8D	1.81(1)									

Table S3. Selected bond distances (Å) for compound **Cu_8L_4-(DMAc).**

Cu_8L_4-(DMF)

C10	C9	1.29(7)	C38	C35	1.56(4)	C64	C63	1.39(3)	O3	C19	1.27(4)
C10	S3	1.67(4)	C39	O20	1.27(4)	C65	C66	1.39(4)	O4	C19	1.28(4)
C11	C11	1.23(1)	C39	C40	1.60(4)	C65	C68	1.63(3)	O5	C57	1.26(4)
C11	S3	1.83(2)	C3B	O1B	1.2(1)	C66	C67	1.39(3)	O6	C57	1.27(4)
C13	C14	1.39(5)	C3B	N1B	1.33(6)	C67	C62	1.39(3)	O9	C20	1.26(5)
C13	C12	1.53(5)	C4	C3	1.44(4)	C7	C6	1.38(5)	S1	C9	1.71(5)
C14	C15	1.39(4)	C40	C45	1.39(4)	C70	C75	1.39(5)	S1	C8	1.82(4)
C16	C17	1.39(4)	C41	C40	1.39(3)	C70	C69	1.58(5)	S10	C58	1.77(4)
C16	C15	1.39(5)	C42	C41	1.39(3)	C71	C70	1.38(5)	S11	C47	1.59(4)
C17	C18	1.39(4)	C43	C42	1.39(4)	C72	C71	1.39(5)	S11	C49	1.82(2)
C18	C13	1.39(5)	C43	C44	1.39(4)	C73	C72	1.38(5)	S12	C46	1.78(4)
C19	C16	1.62(4)	C43	C46	1.56(4)	C73	C74	1.39(5)	S12	C47	1.86(3)
C2	C7	1.42(6)	C45	C44	1.39(4)	C75	C74	1.39(5)	S13	C50	1.81(5)
C21	C22	1.39(4)	C47	C48	1.34(5)	C76	O11	1.27(4)	S13	C48	1.82(4)
C21	C20	1.42(5)	C48	S14	1.73(3)	C76	O12	1.27(5)	S14	C49	1.75(3)
C22	C23	1.39(4)	C5	C6	1.24(7)	C76	C73	1.44(5)	S15	C60	1.82(4)
C24	C25	1.39(4)	C5	C4	1.35(7)	C9	S2	1.77(5)	S16	C69	1.79(6)
C24	C23	1.39(4)	C5	C8	1.75(5)	Cu5	O15	1.90(2)	S2	C11	1.76(2)
C24	C27	1.60(4)	C50	C51	1.53(5)	Cu5	O1	1.87(2)	S4	C10	1.79(4)
C25	C26	1.39(3)	C51	C52	1.39(4)	Cu5	O19	1.91(2)	S4	C12	1.87(4)
C26	C21	1.39(3)	C52	C53	1.39(4)	Cu5	O18	1.92(2)	S5	C29	1.65(3)
C28	C29	1.39(4)	C53	C54	1.39(4)	Cu5	O22	2.07(2)	S5	C31	1.76(3)
C28	S7	1.76(3)	C55	C56	1.39(3)	Cu5	Cu6	2.638(8)	S6	C29	1.69(3)
C2B	N1B	1.44(6)	C55	C54	1.39(4)	Cu6	O17	1.90(2)	S7	C30	1.85(2)
C3	C2	1.44(6)	C56	C51	1.39(4)	Cu6	O2	1.90(2)	S8	C28	1.73(3)
C30	C30	1.15(1)	C57	C54	1.44(4)	Cu6	O20	1.93(3)	S8	C27	1.77(4)
C30	S6	1.78(2)	C58	C49	1.15(5)	Cu6	O21	2.20(2)	C38	O15	1.25(4)
C31	C32	1.58(4)	C58	S15	1.80(3)	N1B	C1B	1.44(7)	C38	O16	1.26(3)
C32	C33	1.39(3)	C59	C60	1.46(5)	O1	C1	1.26(3)	C62	C63	1.39(4)
C33	C34	1.39(3)	C59	S10	1.58(5)	O10	C20	1.26(4)	C64	C65	1.39(3)
C35	C36	1.39(3)	C59	S9	1.87(6)	O15	Cu5	1.90(2)	O19	C39	1.26(3)
C35	C34	1.39(3)	C60	S16	1.60(4)	O16	Cu6	1.92(2)	O2	C1	1.27(3)
C36	C37	1.39(4)	C61	C62	1.66(4)	O17	C68	1.27(3)			
C37	C32	1.39(3)	C61	S9	1.66(4)	O18	C68	1.26(4)			

Table S4. Selected bond distances (Å) for compound **Cu_8L_4-(DMF).**

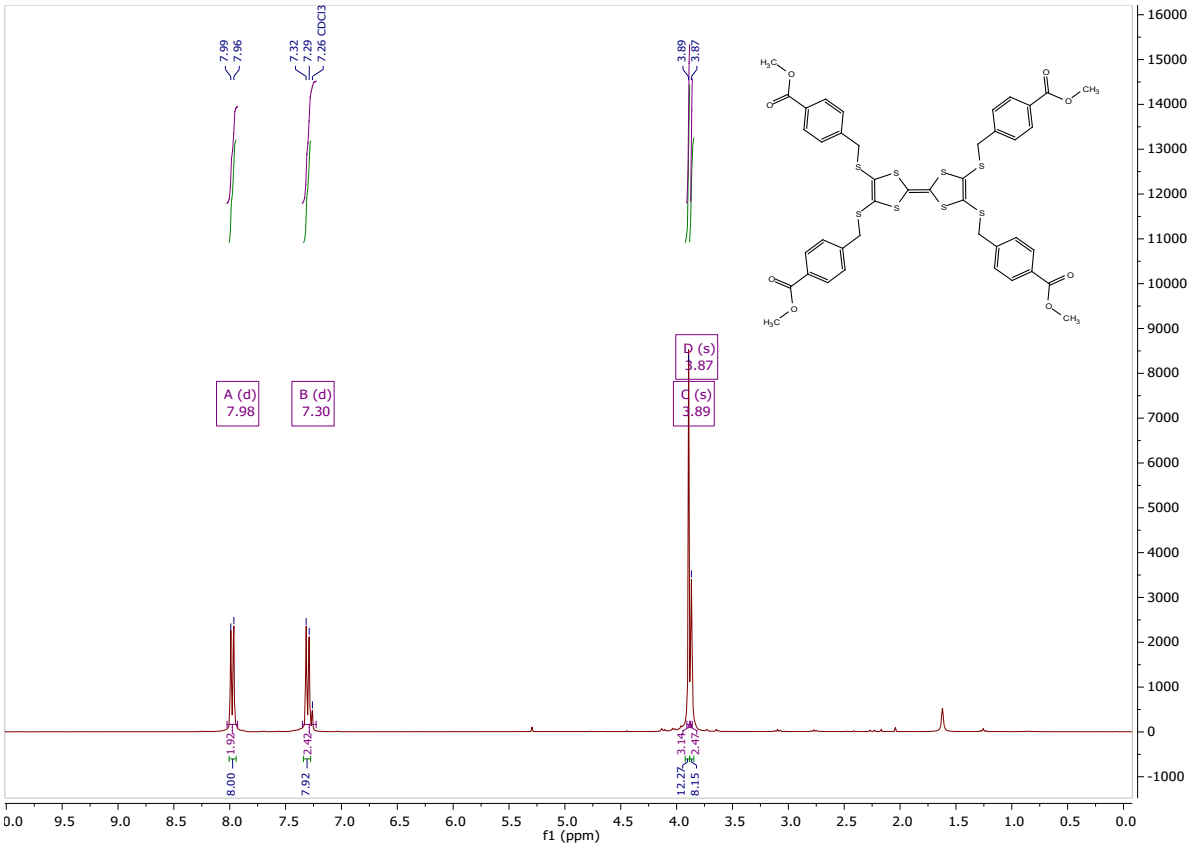


Figure S1. ^{1}H NMR (300 MHz, $CDCl_3$) spectra of **2**

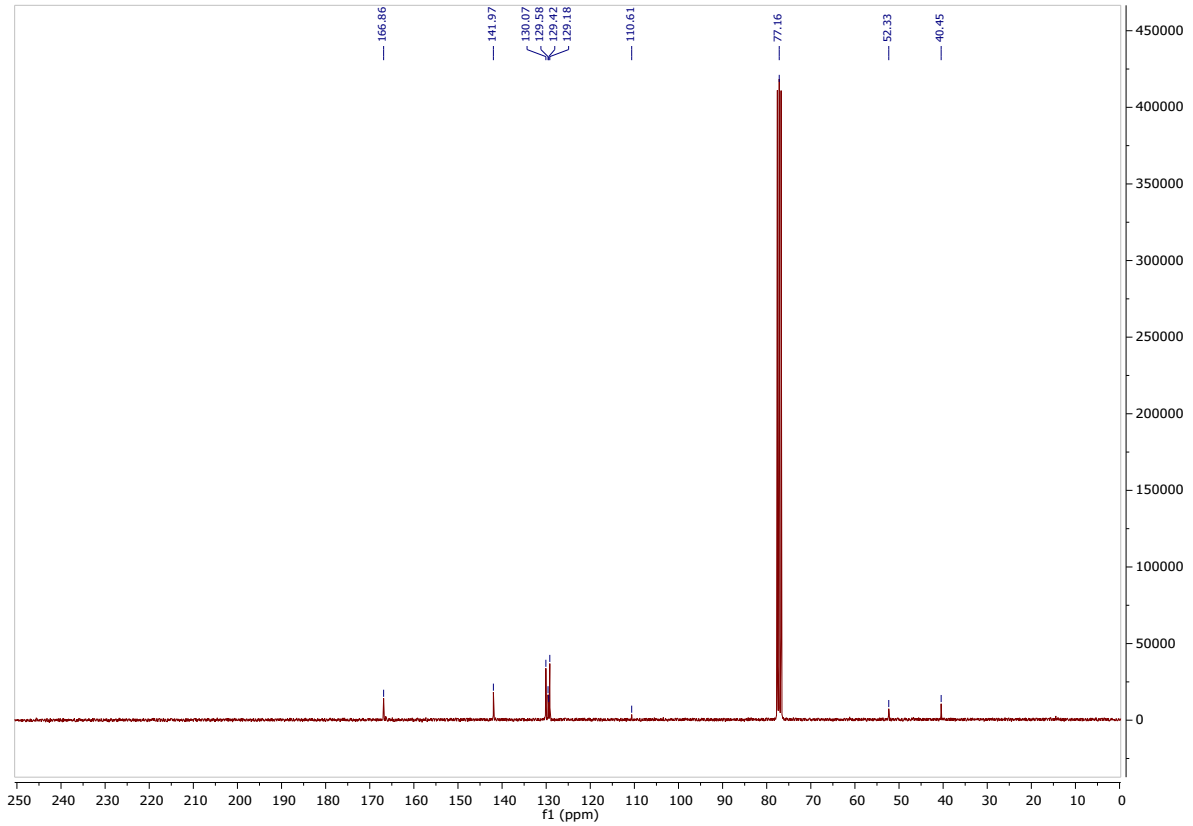


Figure S2. ^{13}C NMR (75 MHz, $CDCl_3$) spectra of **2**

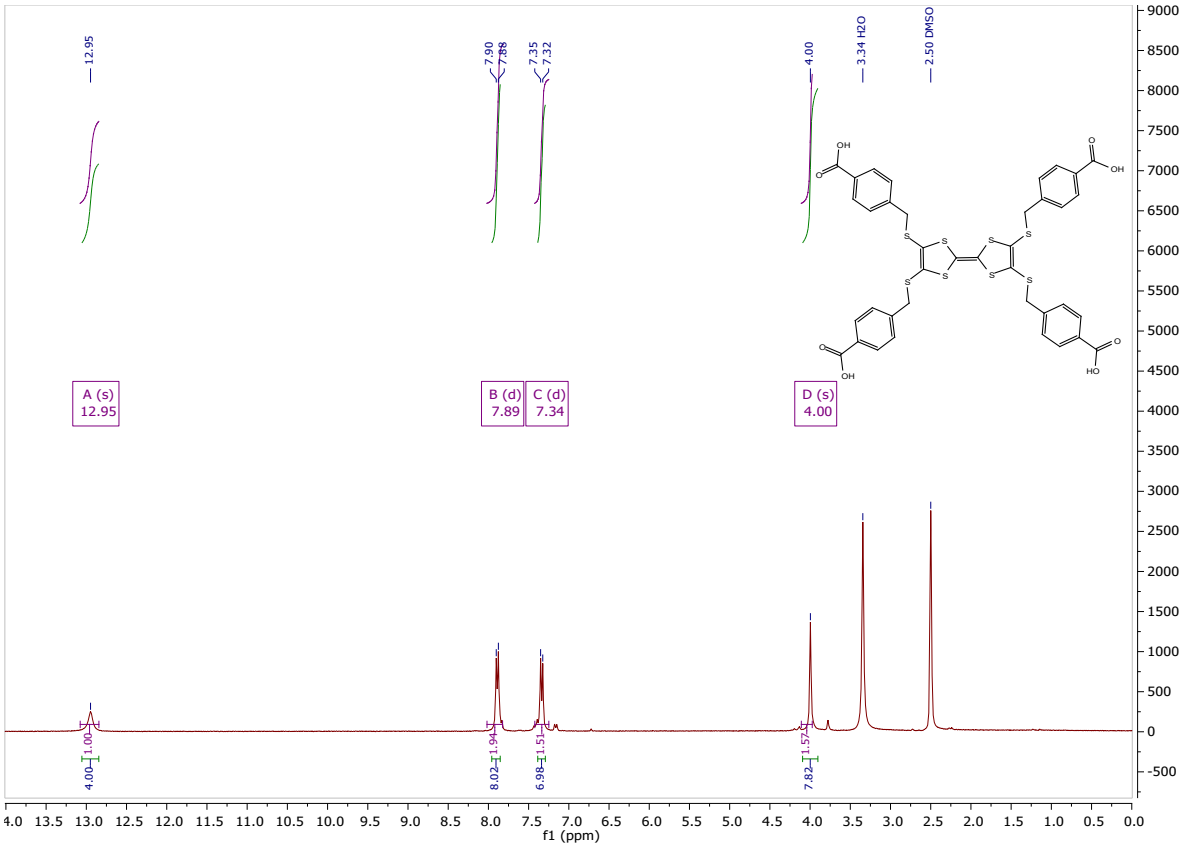


Figure S3. ^{1}H NMR (300 MHz, DMSO-d_6) spectra of **L**

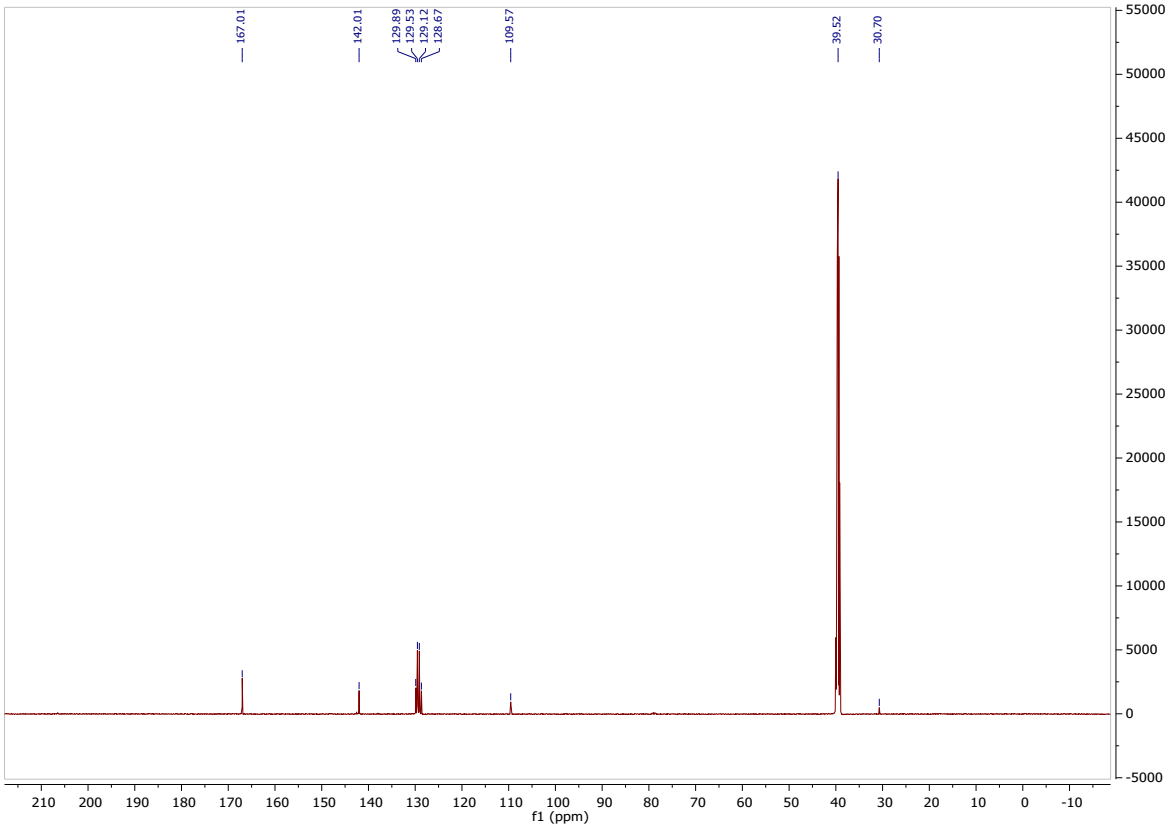


Figure S4. ^{13}C NMR (75 MHz, DMSO-d_6) spectra of **L**

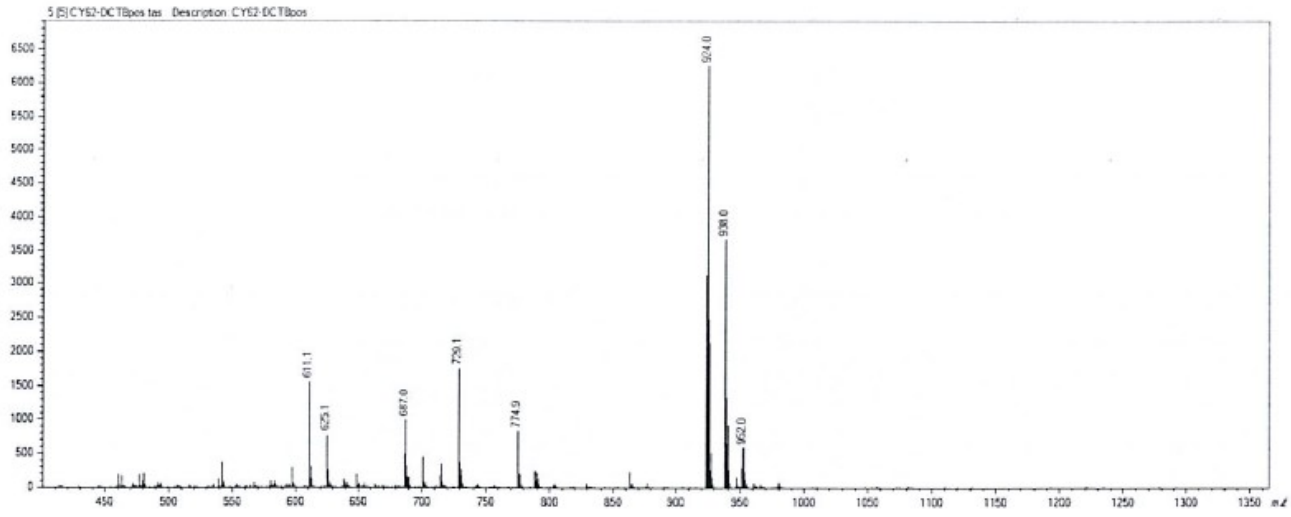
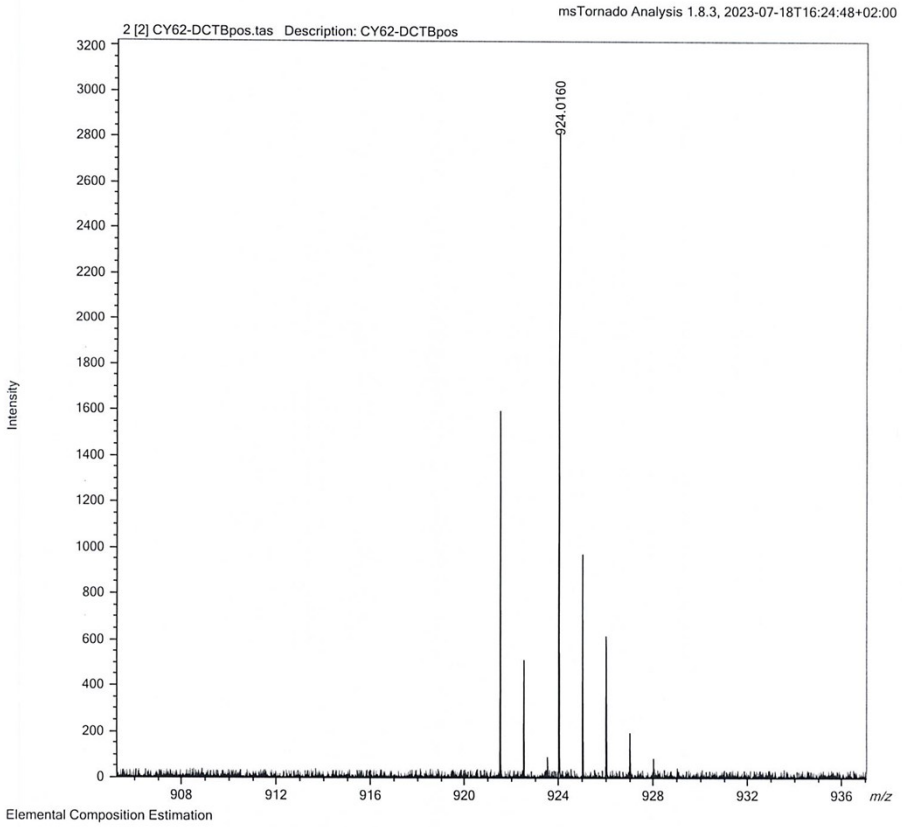


Figure S5. LRMS of **2**.



Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
924.01598 ± 0.00185	2.0 ppm	Odd	+1	-0.5 - 200.0	100

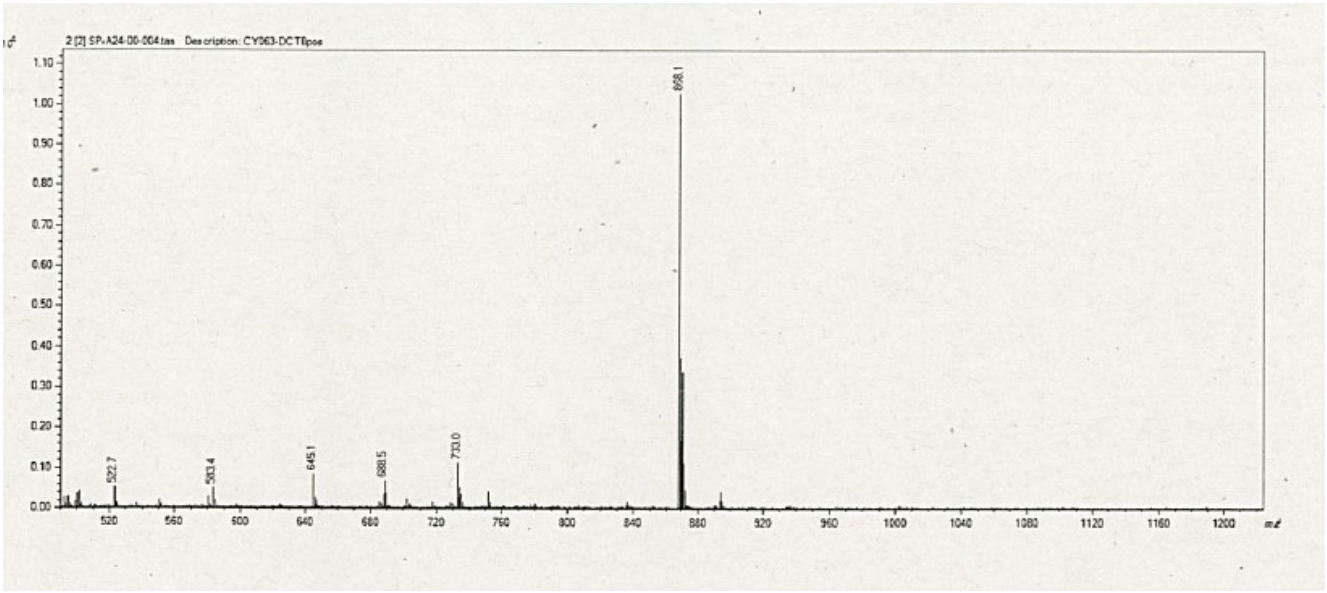
Elements

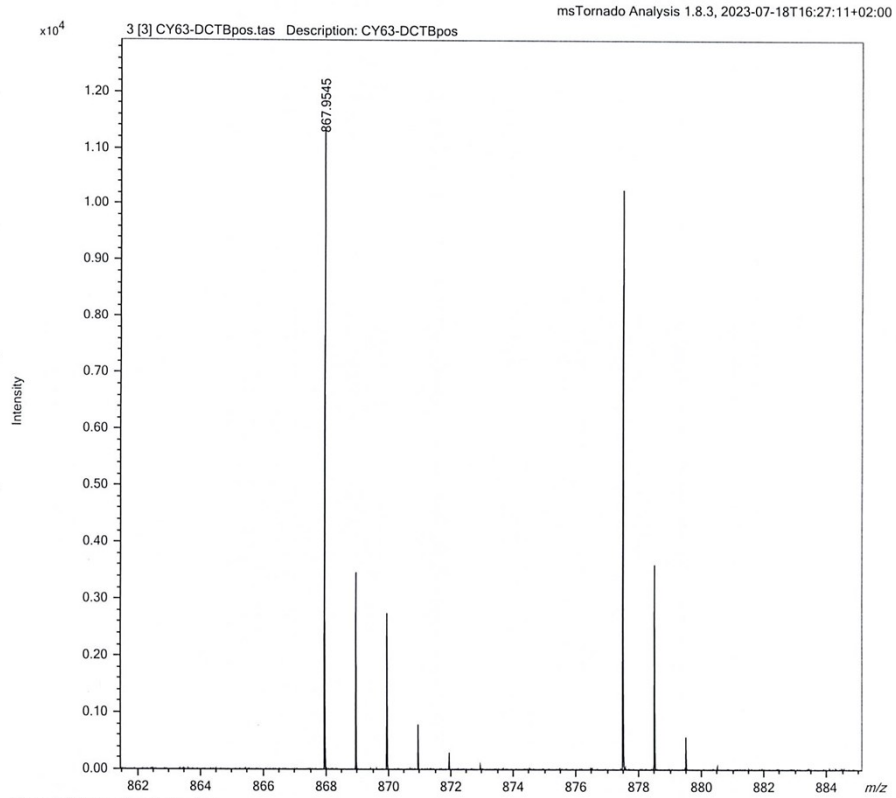
C	H	N	O	Na	S
0 - 45	0 - 100	0 - 0	0 - 10	0 - 0	0 - 10

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C42 H36 O8 S8	924.01704	25.0	0.00106	-0.00106	-1.14

Figure S6. HRMS of **2**.





Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
867.95448 ± 0.00043	0.5 ppm	Odd	+1	-0.5 - 200.0	100

Elements

C	H	N	O	Na	S
0 - 45	0 - 100	0 - 0	0 - 10	0 - 0	0 - 10

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C38 H28 O8 S8	867.95443	25.0	0.00005	0.00005	0.06

Figure S8. HRMS of **L**.

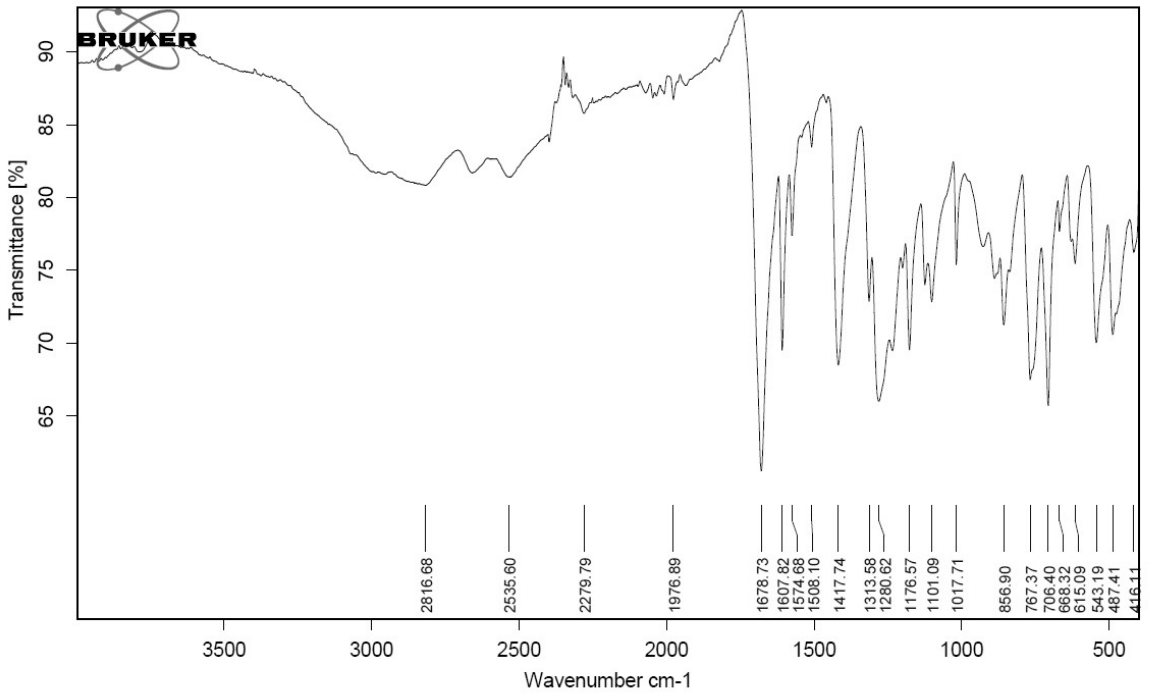


Figure S9. IR spectra of **L**.

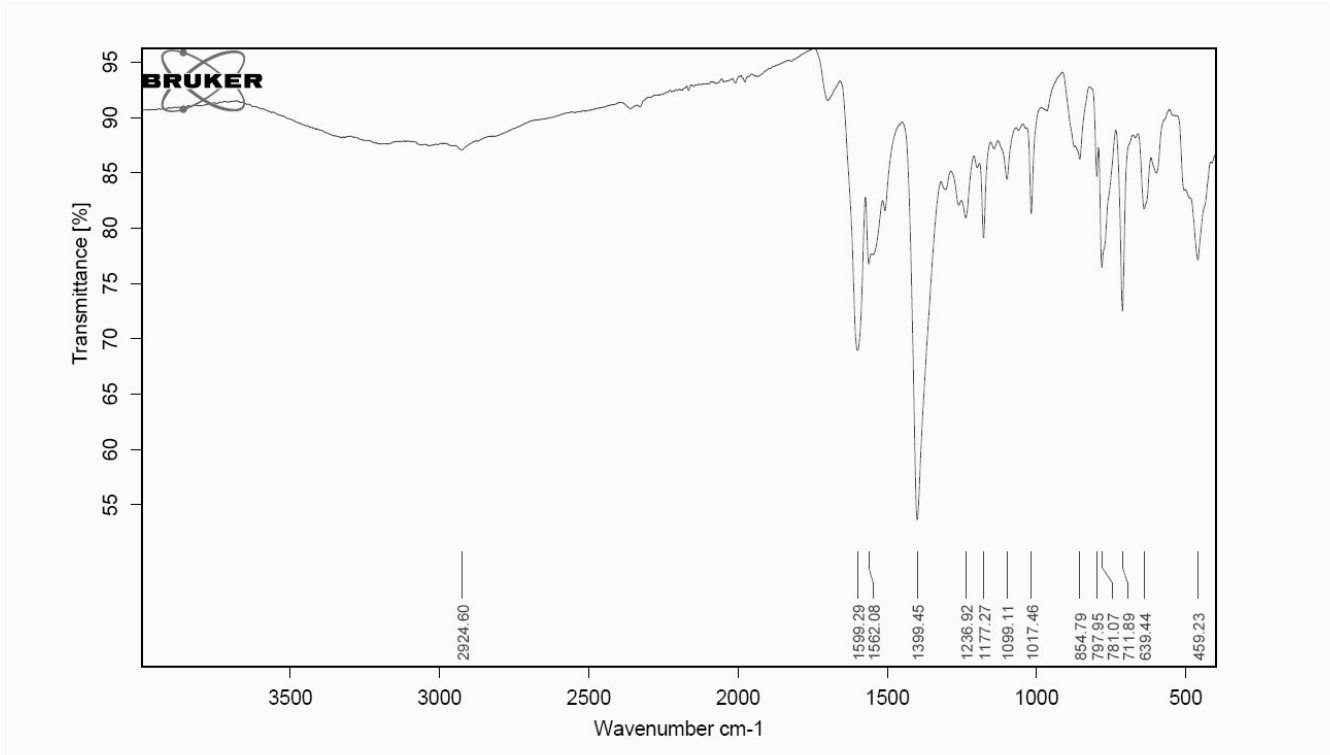


Figure S10. IR spectra of **Cu_8L_4-(DMAc).**

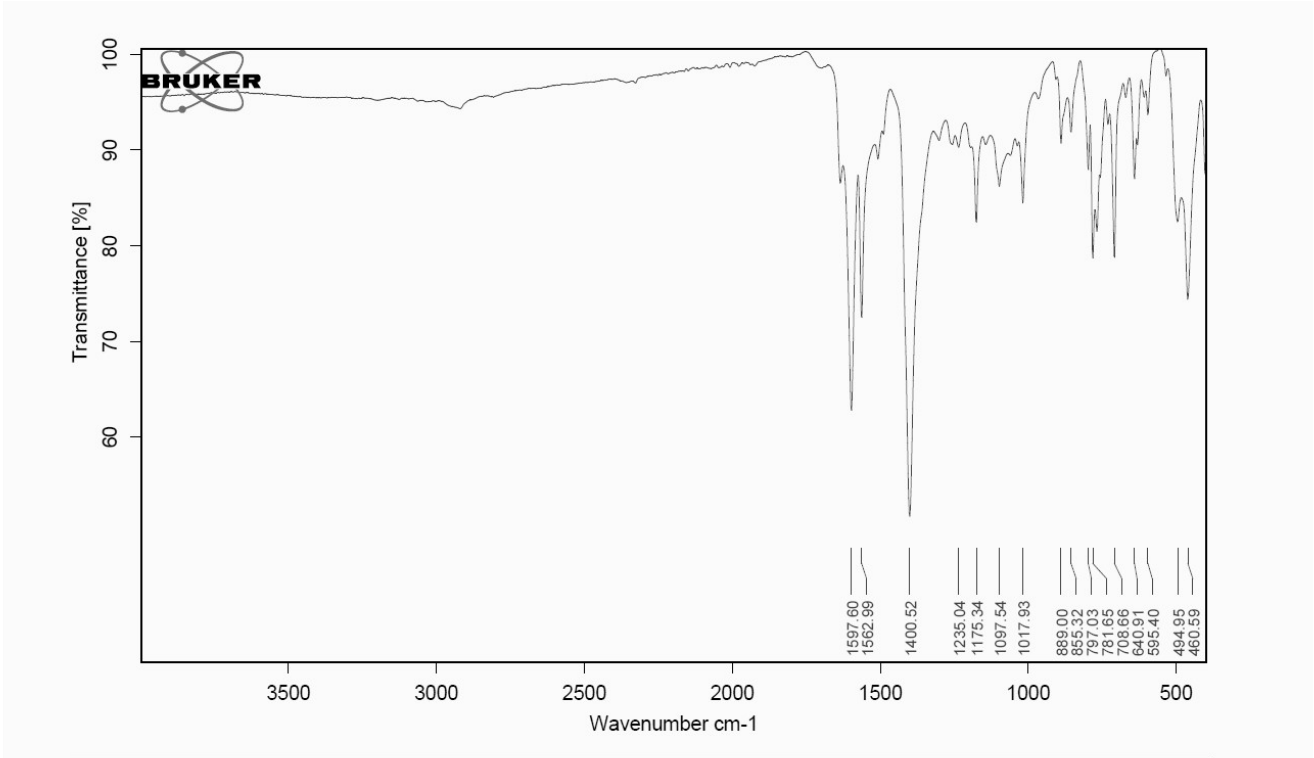


Figure S11. IR spectra of **Cu_8L_4-(DMAc)** after drying**.**

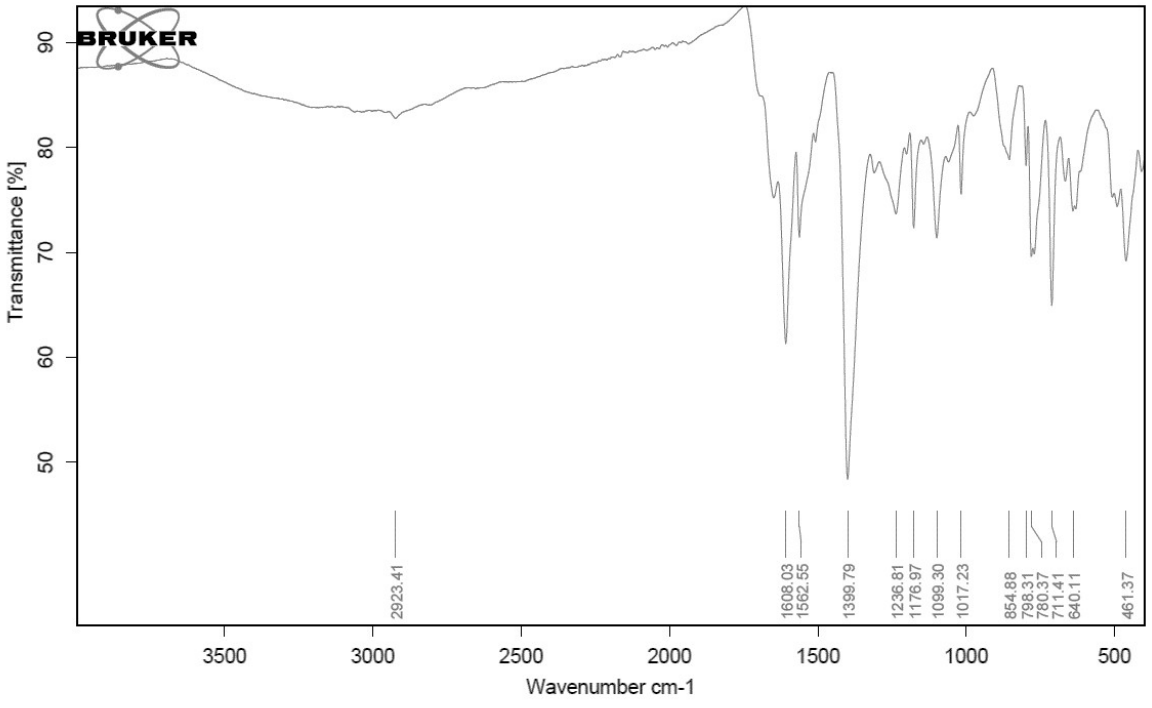


Figure S12. IR spectra of **Cu_8L_4-(DMF)**.

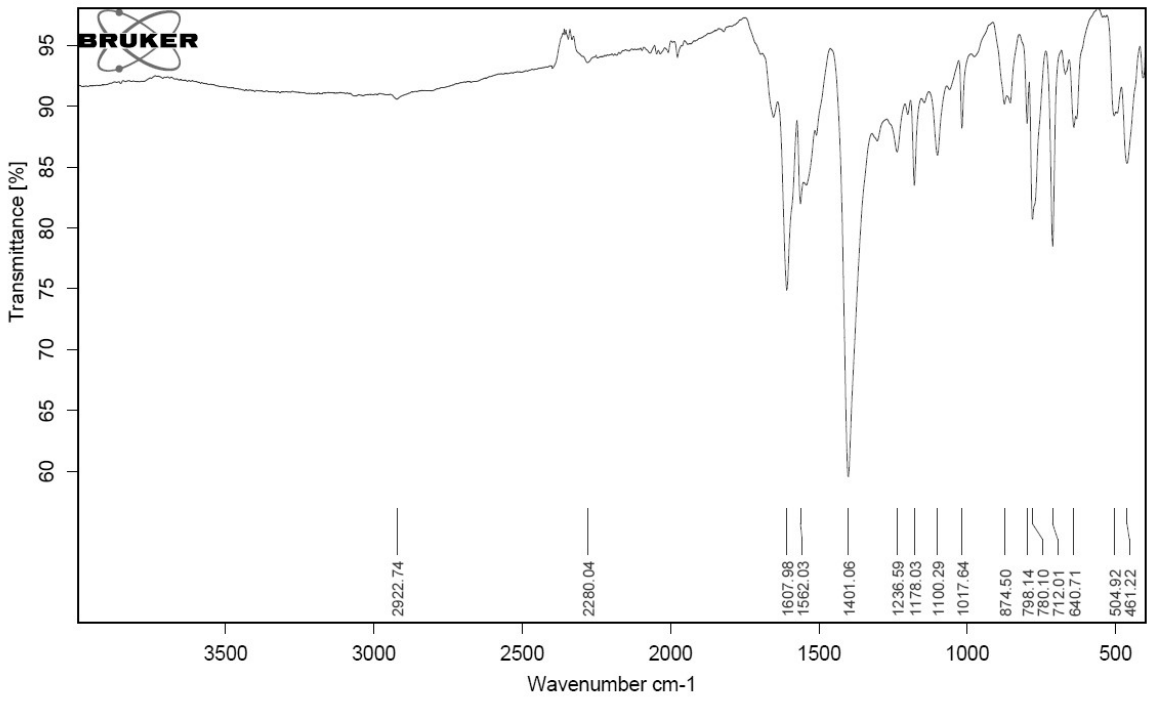


Figure S13. IR spectra of **Cu_8L_4-(DMF)** after drying**.**

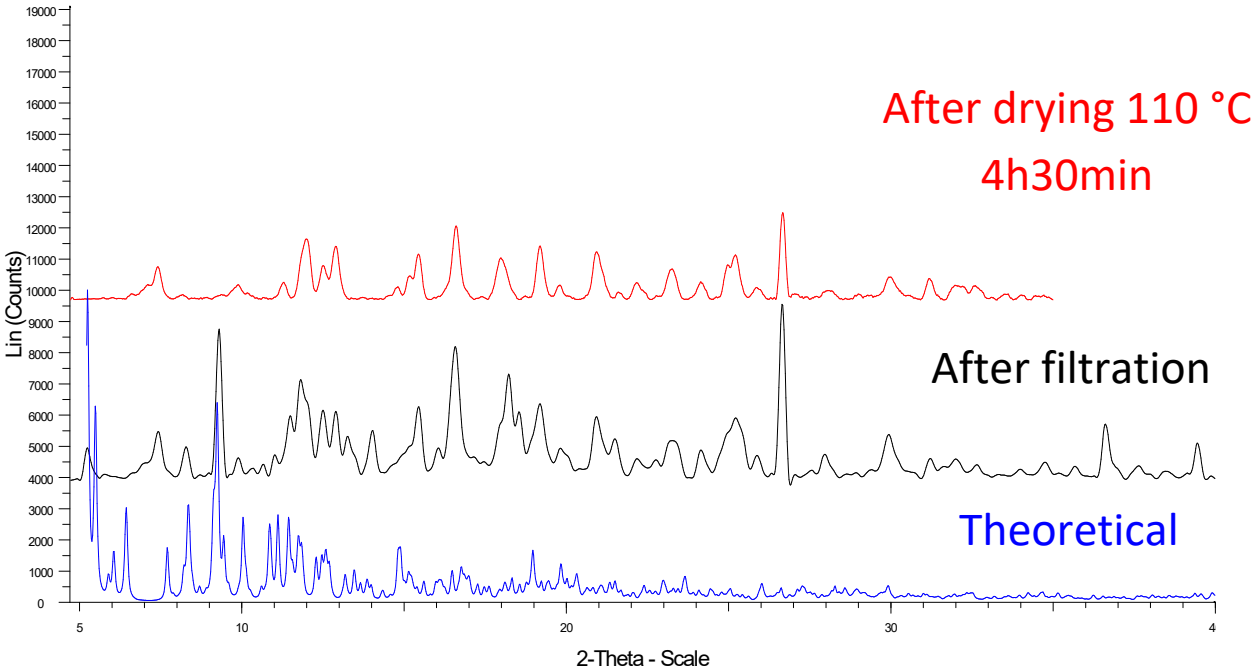


Figure S14. PXRD for **Cu_8L_4-(DMAc)**.

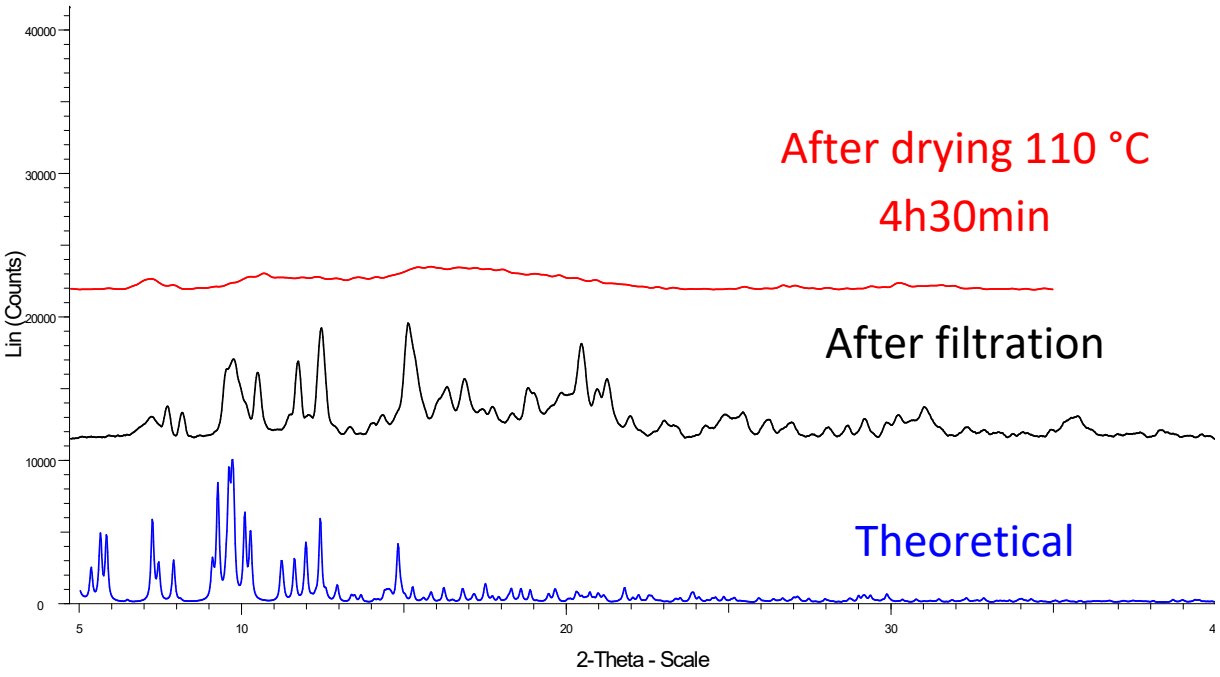


Figure S15. PXRD for **Cu_8L_4-(DMF)**.

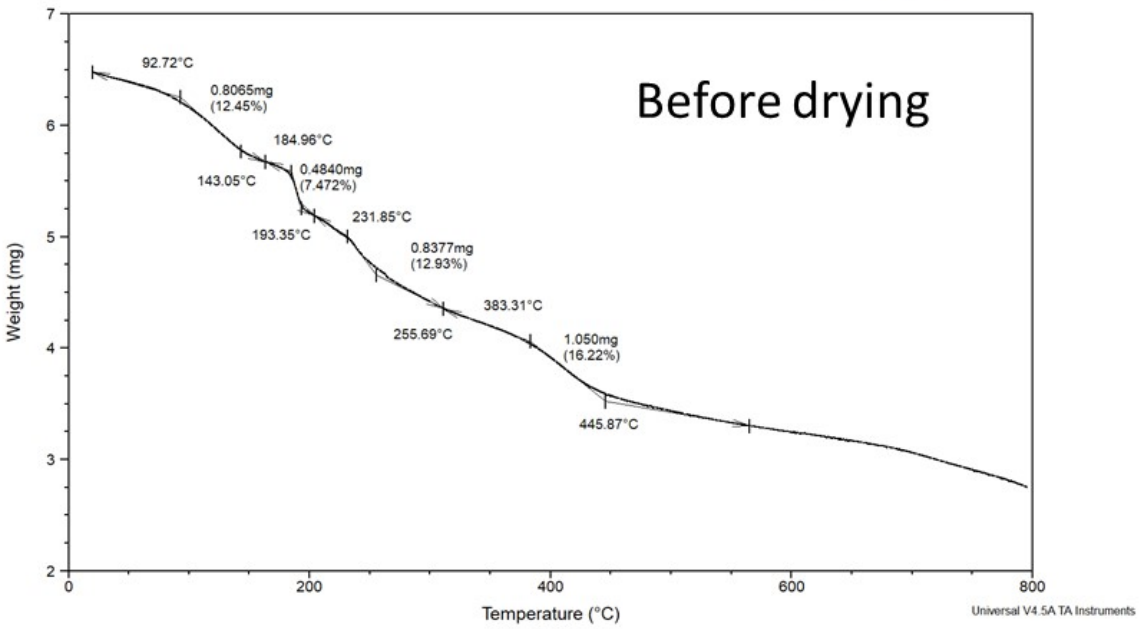


Figure S16. TGA before drying for **Cu_8L_4-(DMAc)**.

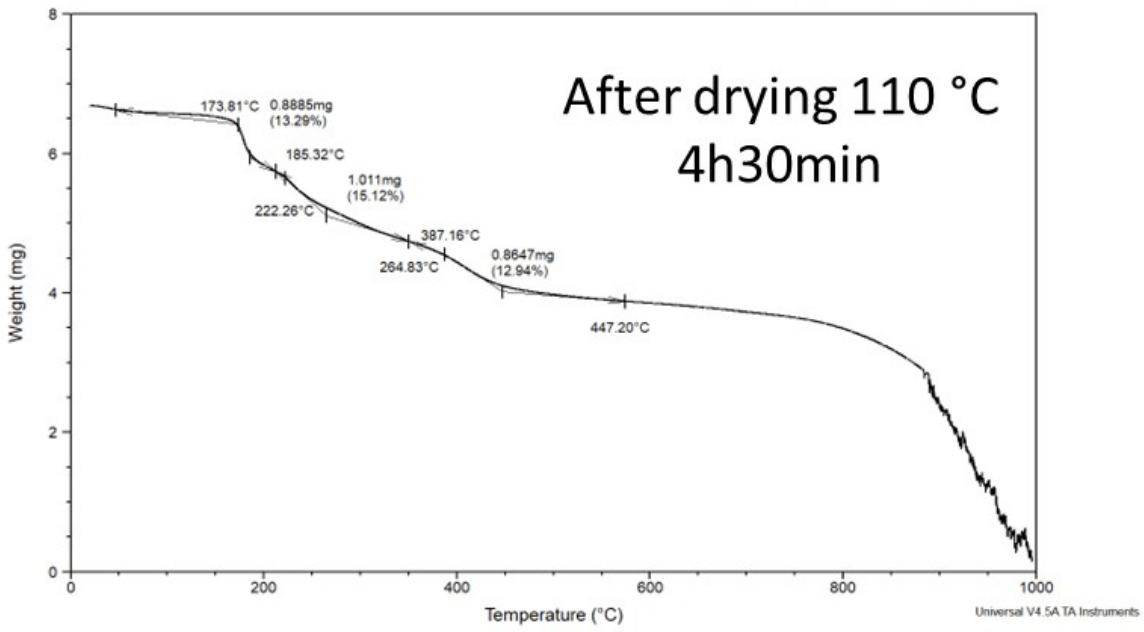


Figure S17. TGA after drying for **Cu_8L_4-(DMAc)**.

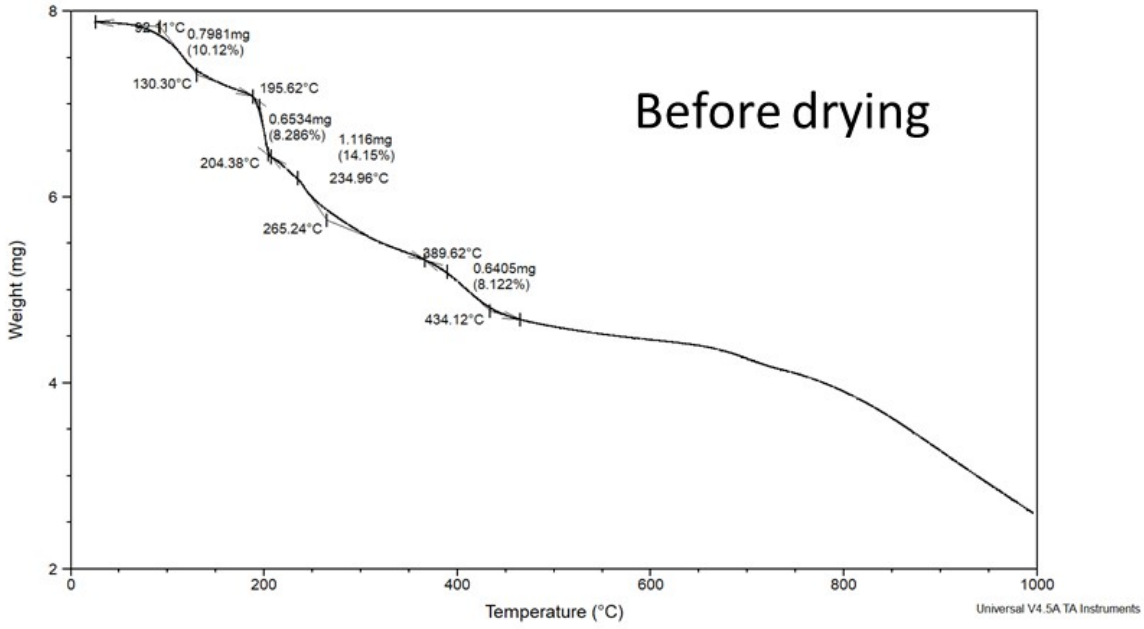


Figure S18. TGA before drying for **Cu_8L_4-(DMF)**.

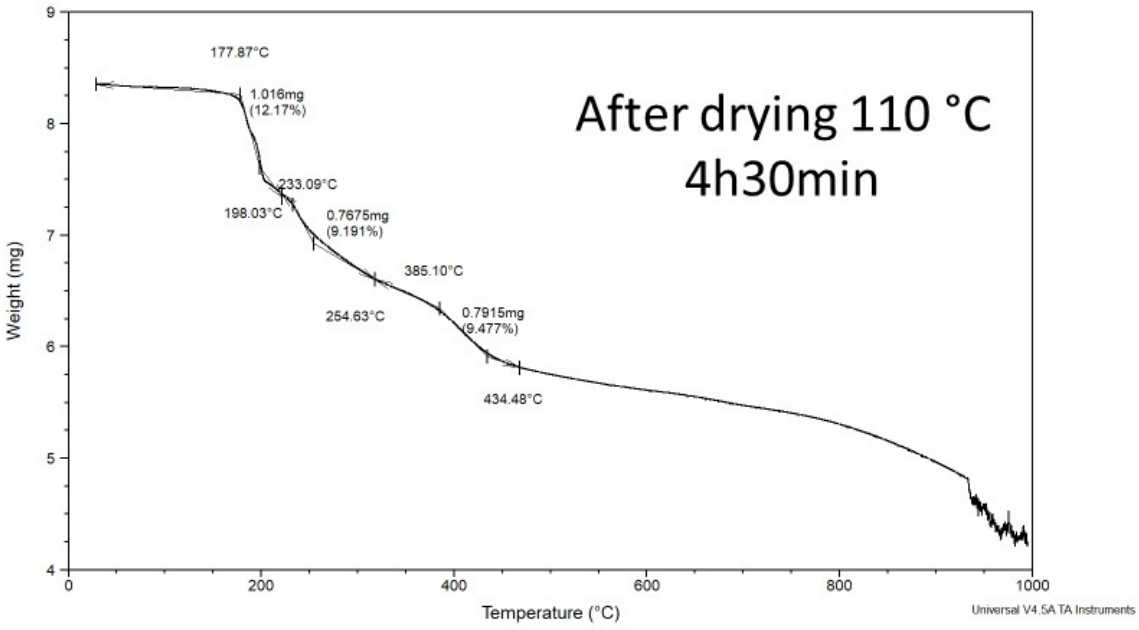


Figure S19. TGA after drying for **Cu_8L_4-(DMF)**.

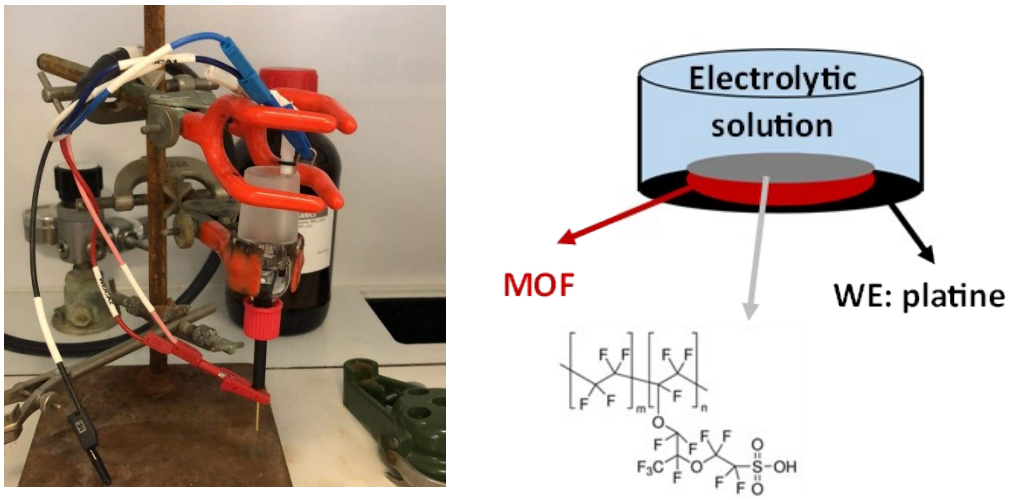


Figure S20. Solid state cyclic voltammetry set-up (left: set-up picture, right: schematic representation).

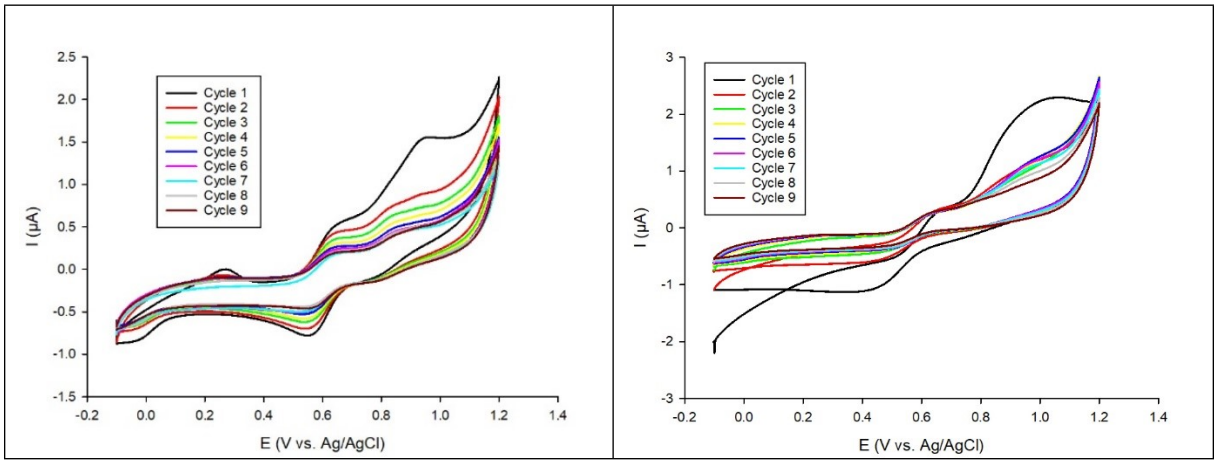


Figure S21. Solid-state cyclic voltammograms for **Cu_8L_4-(DMF)** (left) and **Cu_8L_4-(DMAc)** (right) recorded between -0.1 V and 1.2 V (WE: Pt; CE: Pt wire; RE: Ag/AgCl; electrolyte : 0.1 M $TBAPF_6$ in CH_3CN ; scan rate: 20 $mV.s^{-1}$).

References

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