

Supporting Information

for

Azole-linkers with a mesitylene core: synthesis and characterization

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Synthetic procedures, NMR spectra and crystallographic data

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NMR Spectra

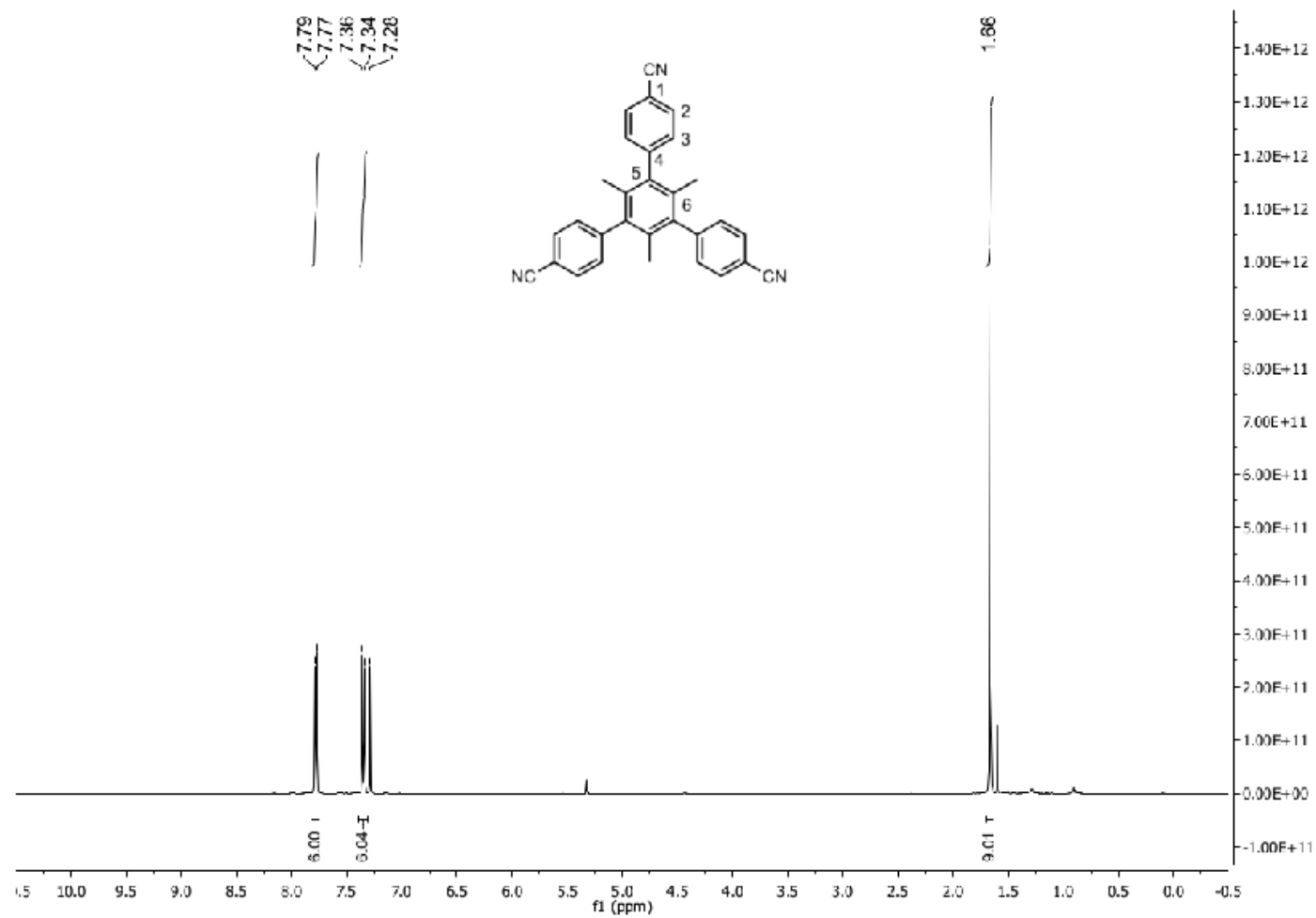


Figure S1 – The ^1H NMR spectrum of **2**, measured in CDCl_3 .

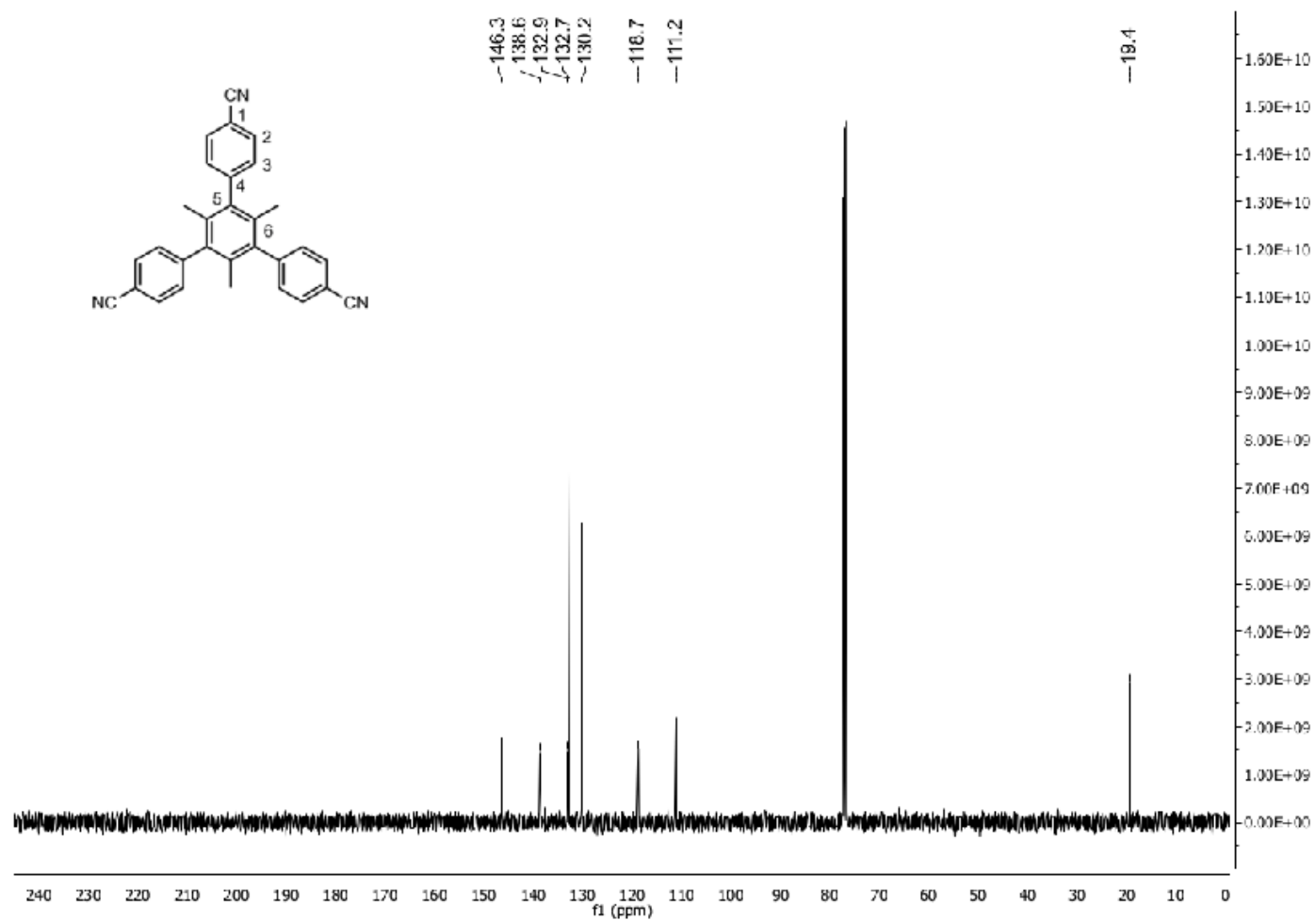


Figure S2 – The ^{13}C NMR spectrum of **2**, measured in CDCl_3 .

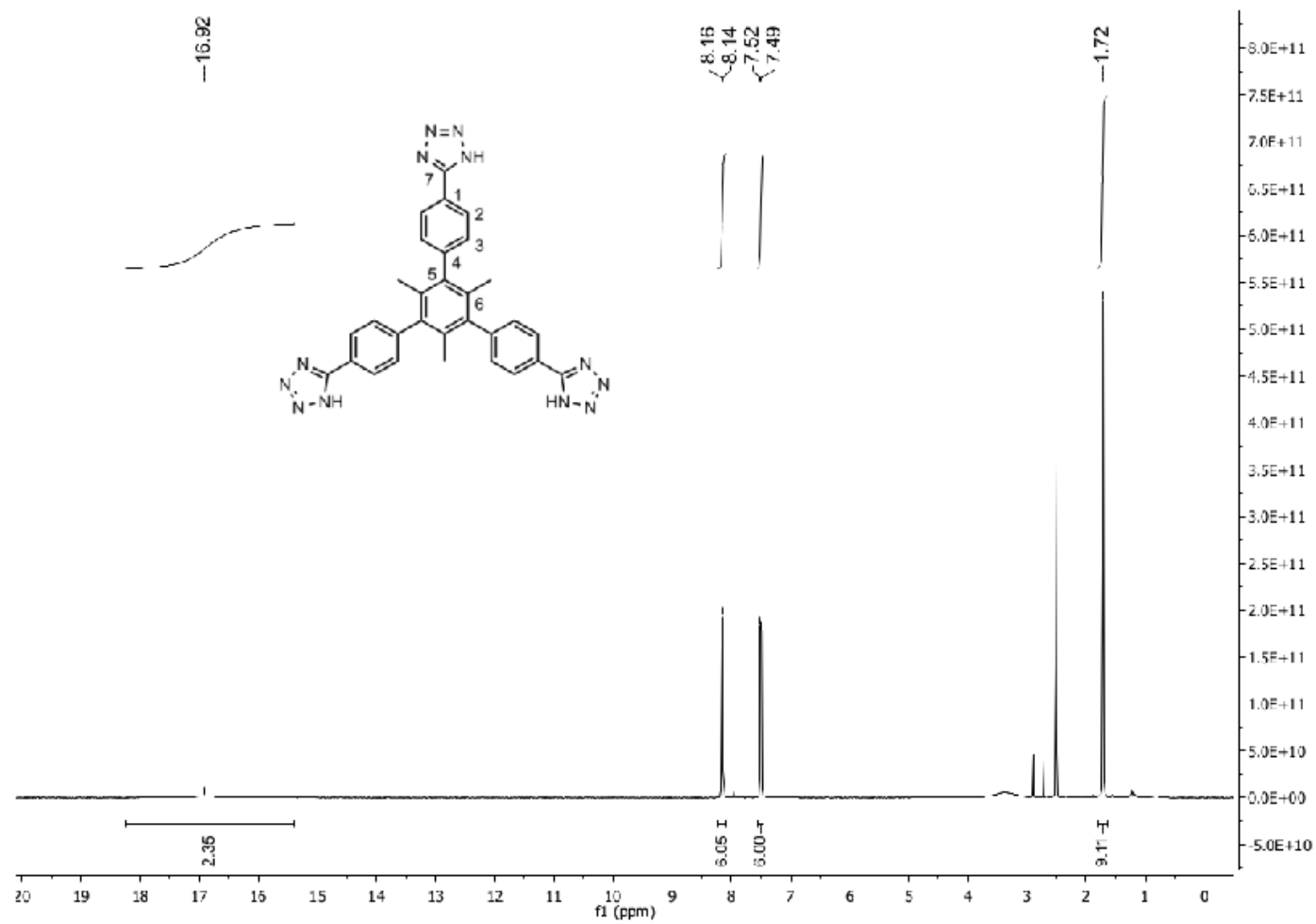


Figure S3 – The ^1H NMR spectrum of **3**, measured in $\text{DMSO}-d_6$.

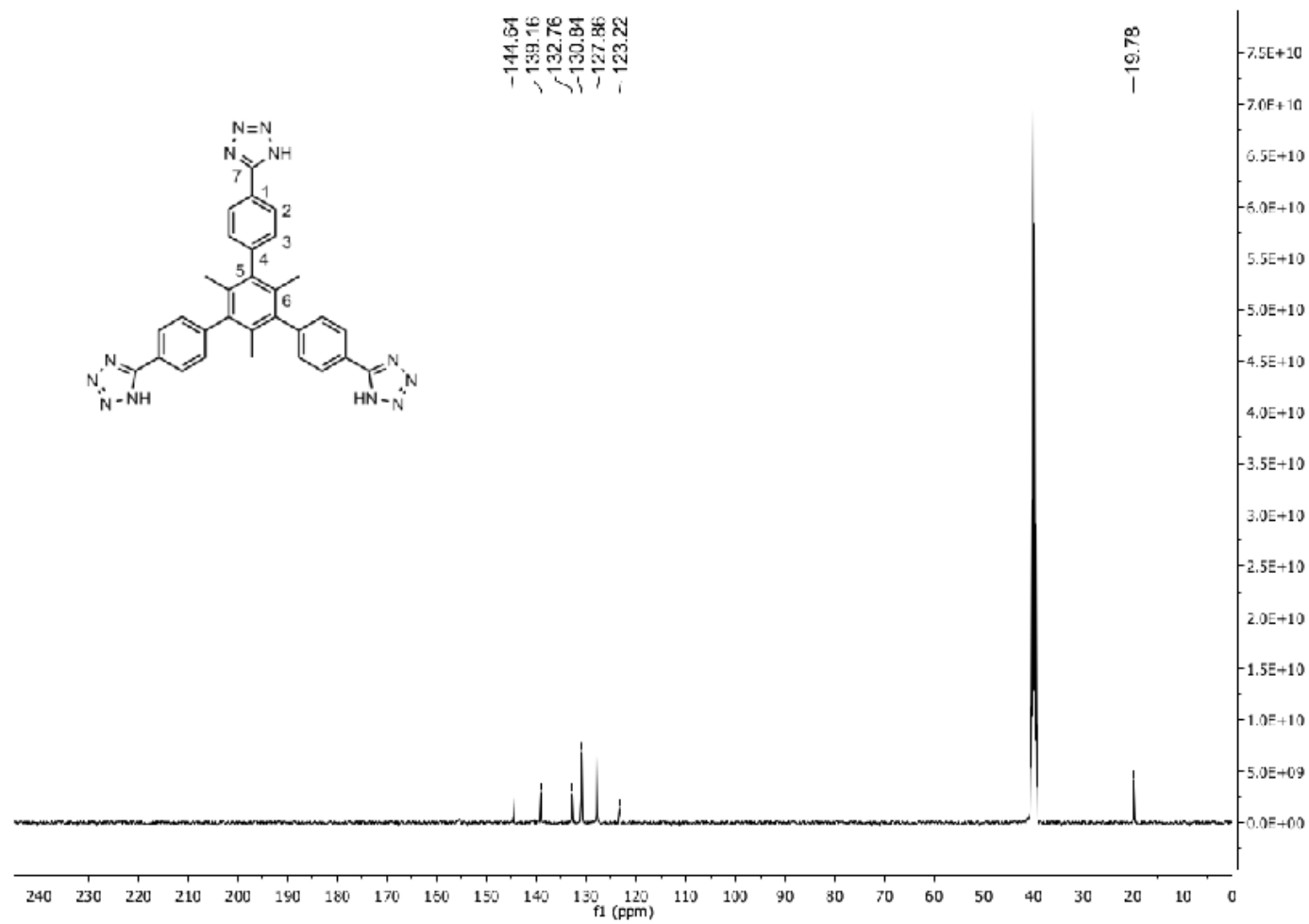


Figure S4 – The ^{13}C NMR spectrum of **3**, measured in $\text{DMSO}-d_6$.

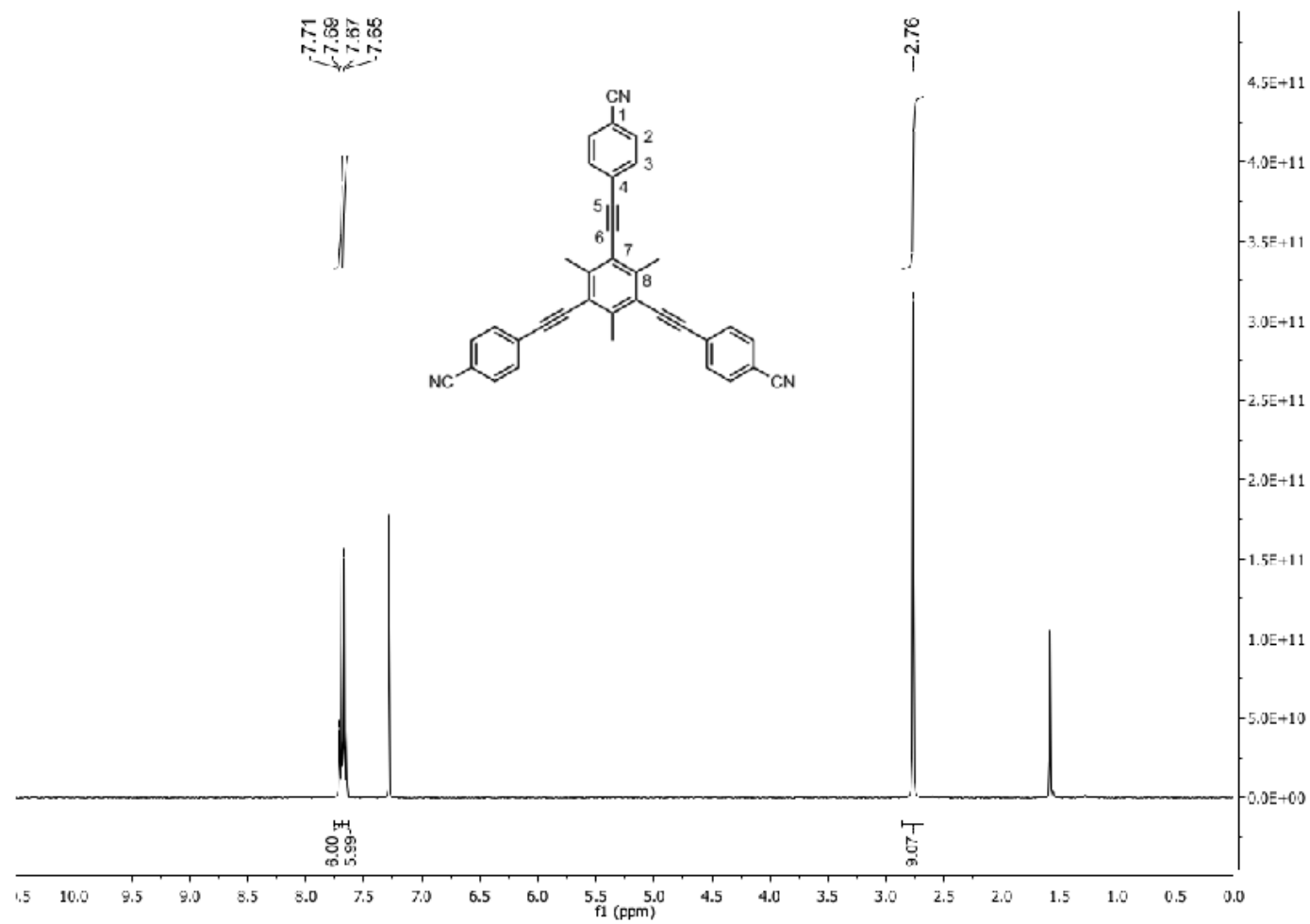


Figure S5 – The ^1H NMR spectrum of **4**, measured in CDCl_3 .

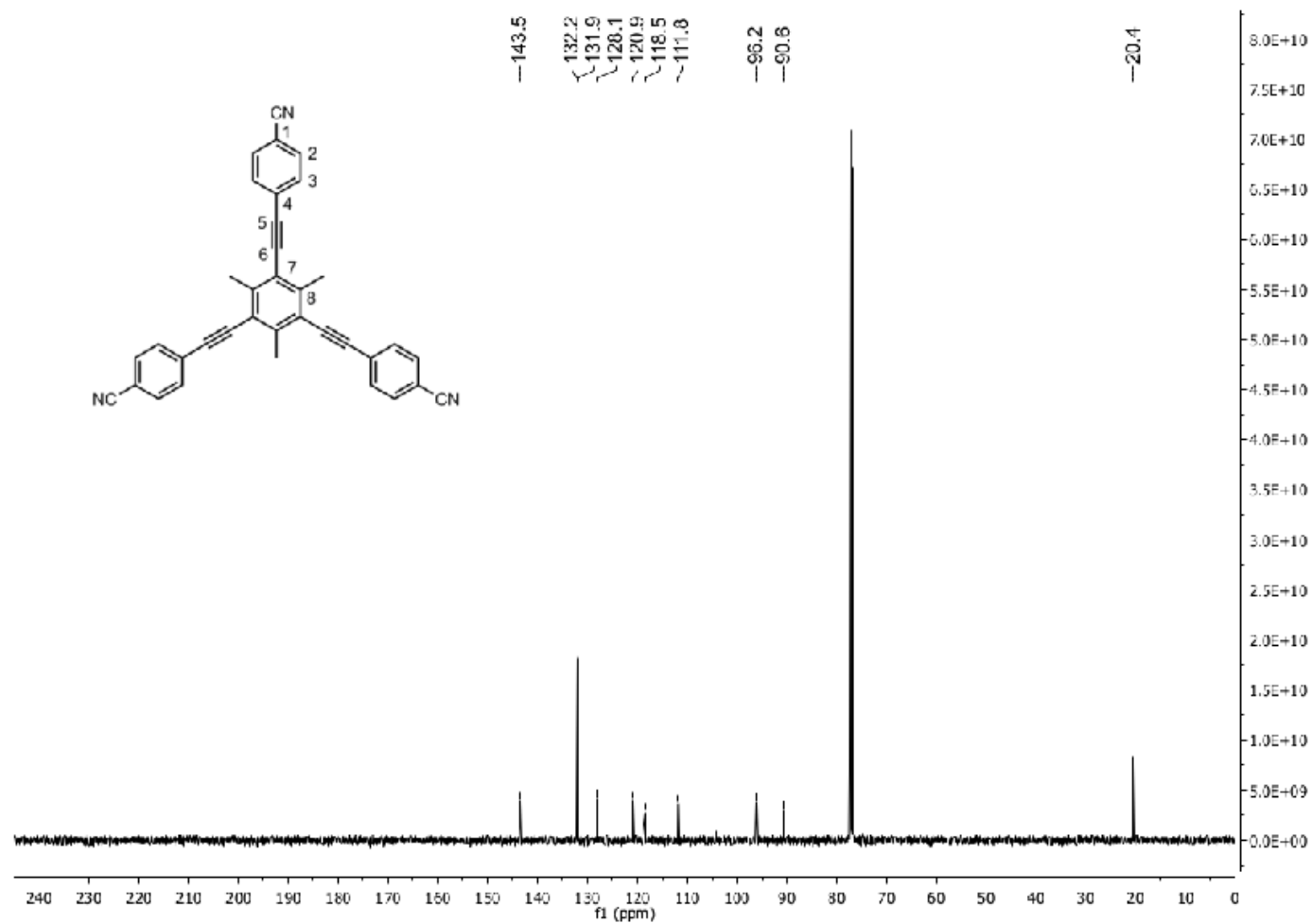


Figure S6 – The ^{13}C NMR spectrum of **4**, measured in CDCl_3 .

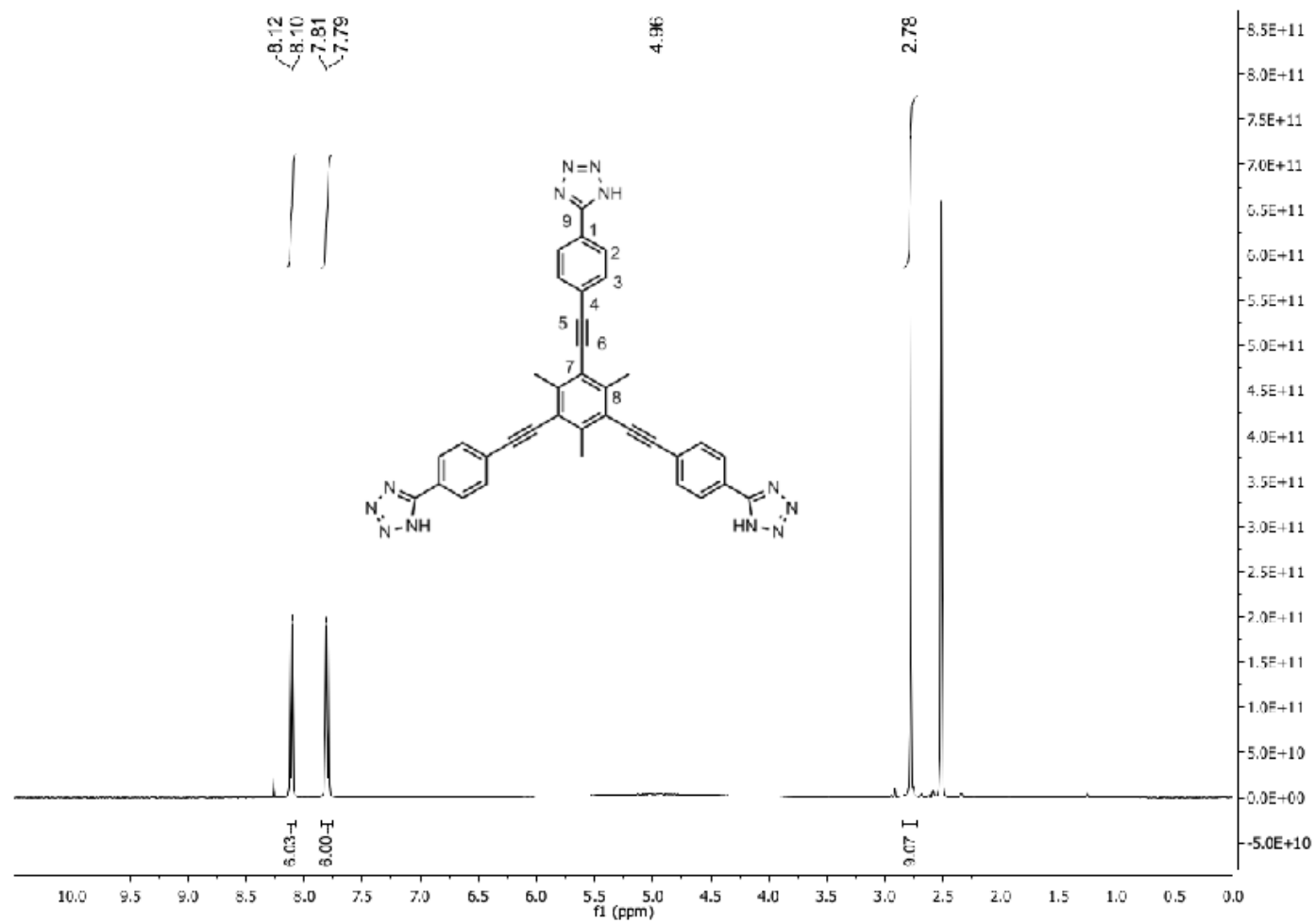


Figure S7 – The ^1H NMR spectrum of **5**, measured in $\text{DMSO-}d_6$.

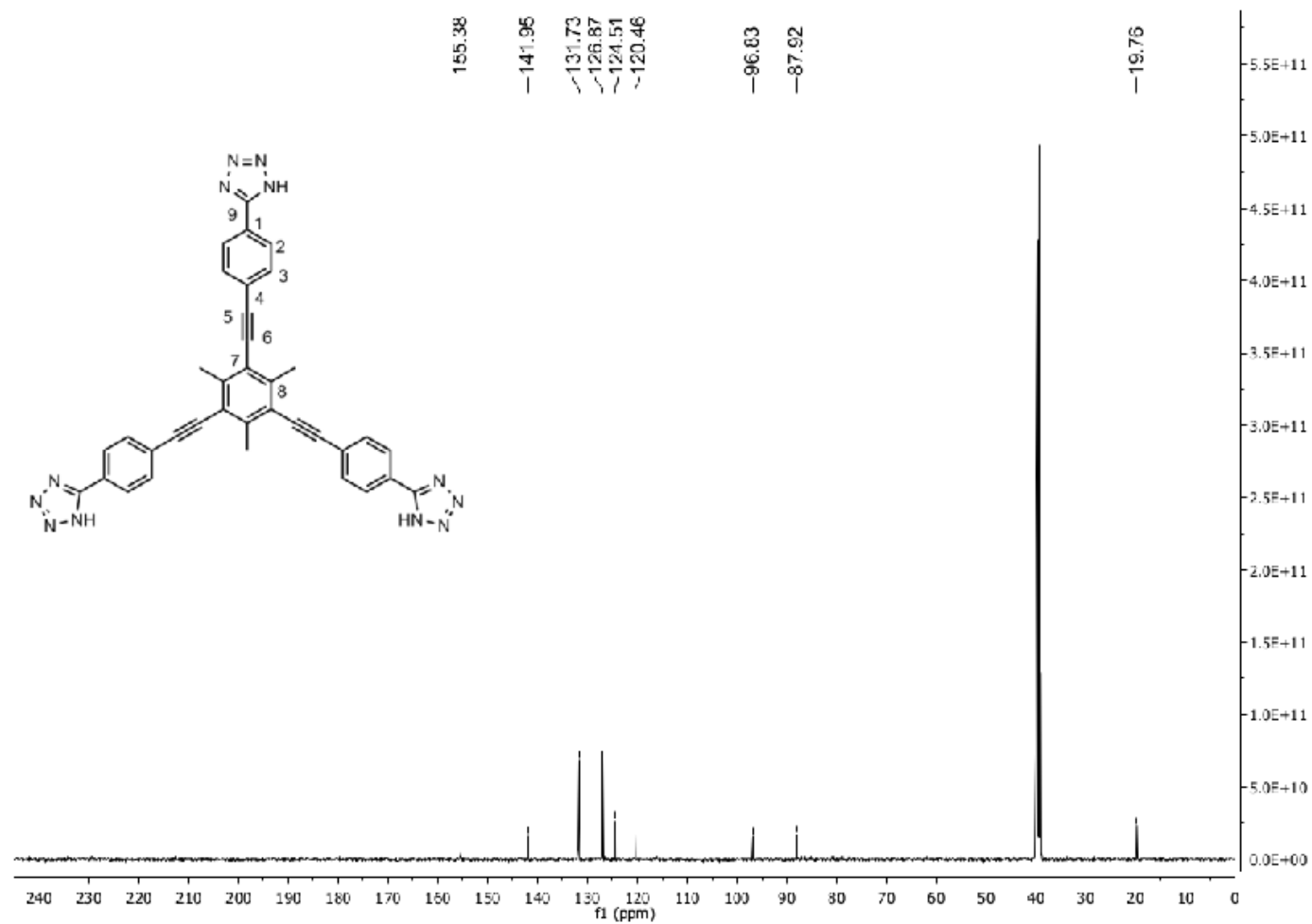


Figure S8 – The ¹³C NMR spectrum of **5**, measured in DMSO-*d*₆.

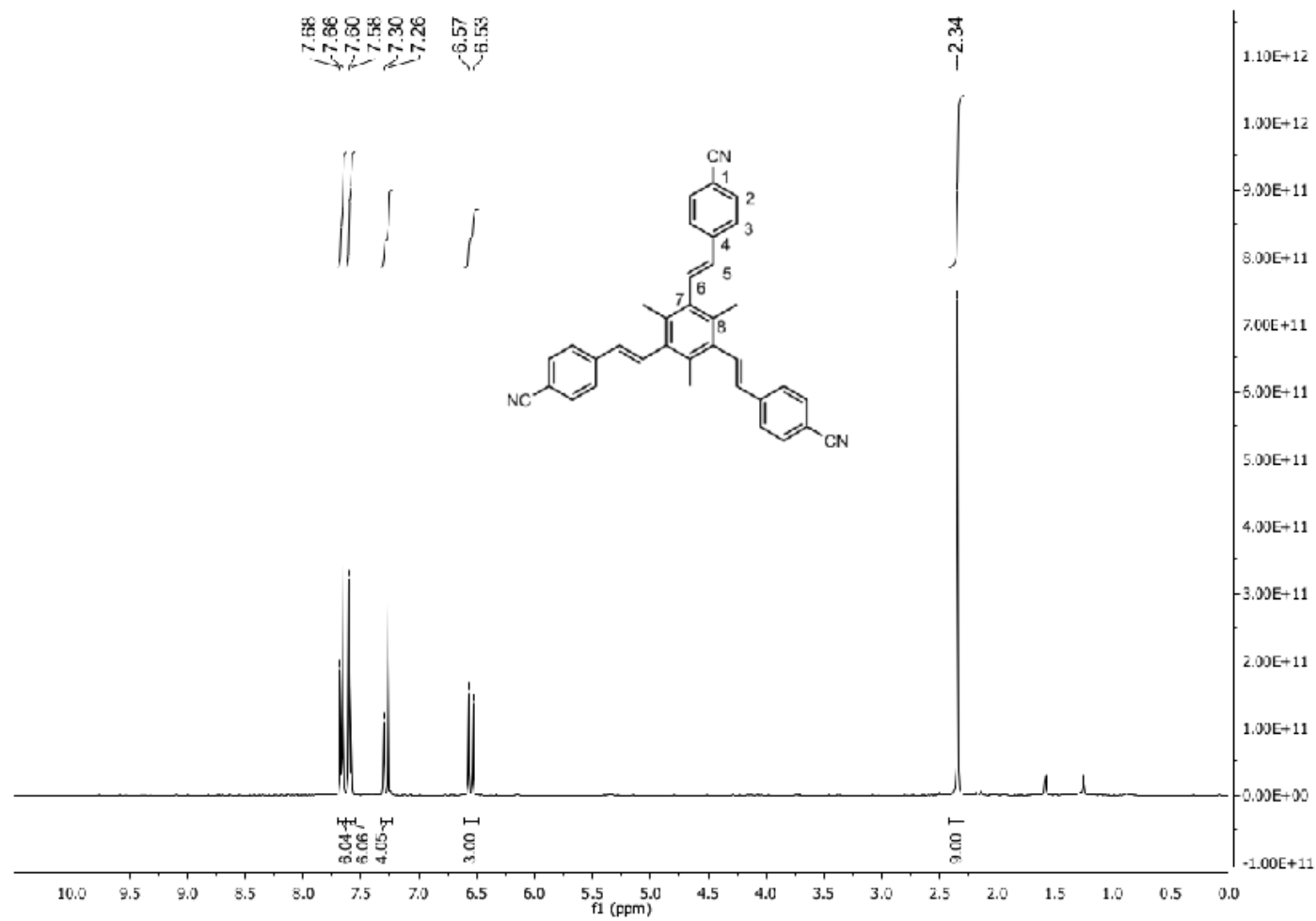


Figure S9 – The ^1H NMR spectrum of **6**, measured in CDCl_3 .

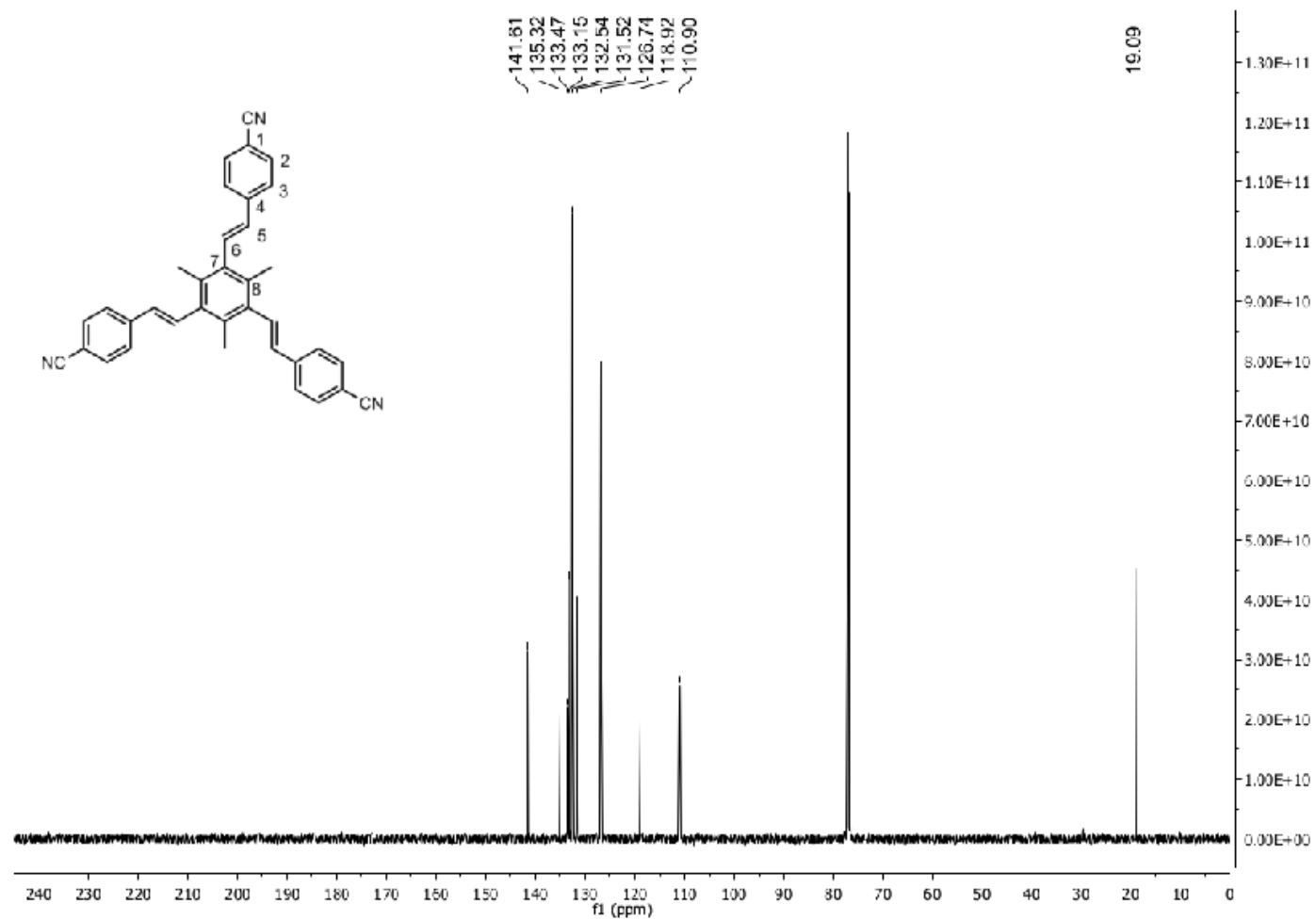


Figure S10 – The ¹³C NMR spectrum of **6**, measured in CDCl₃.

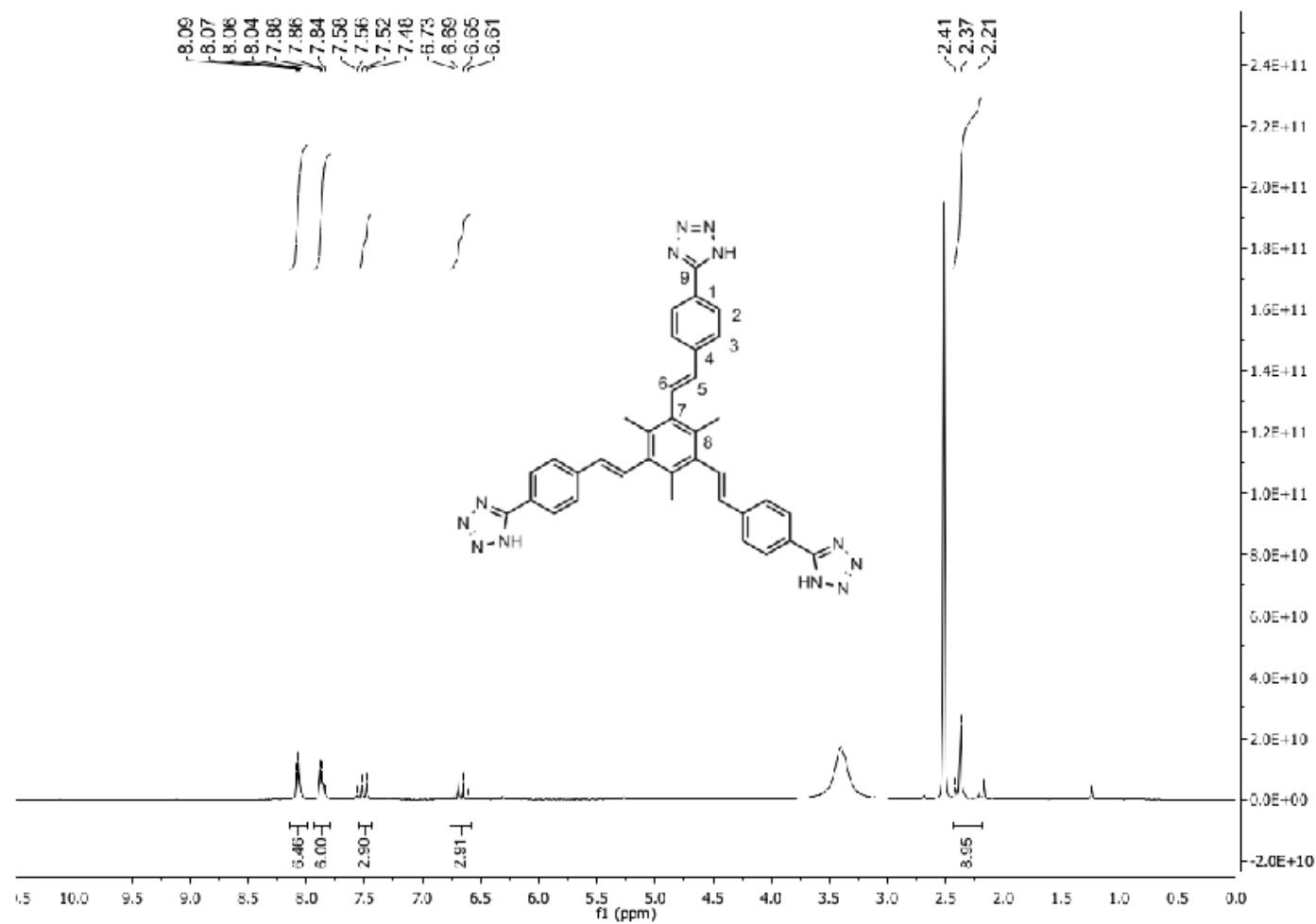


Figure S11 – The ^1H NMR spectrum of **7**, measured in $\text{DMSO-}d_6$.

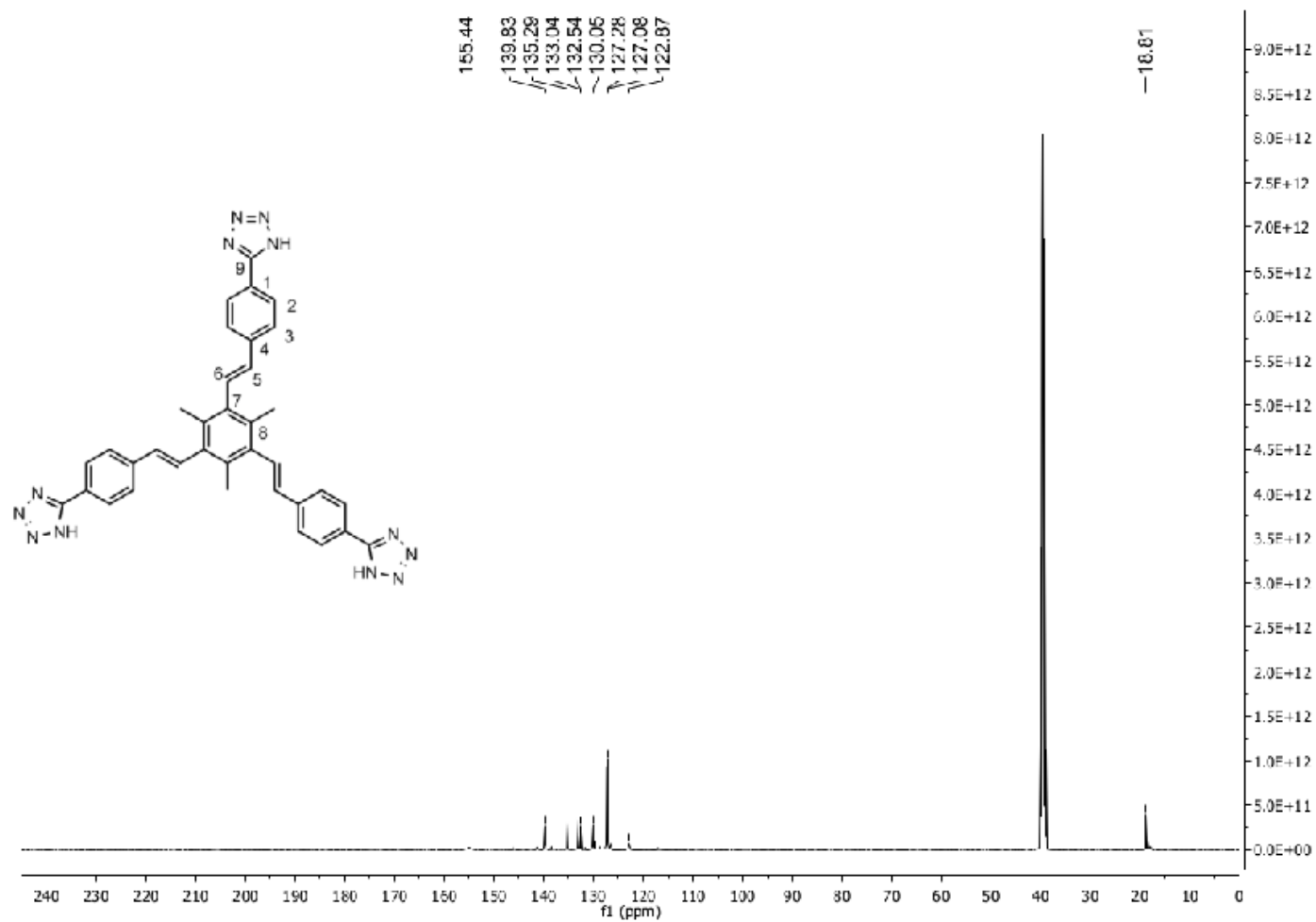
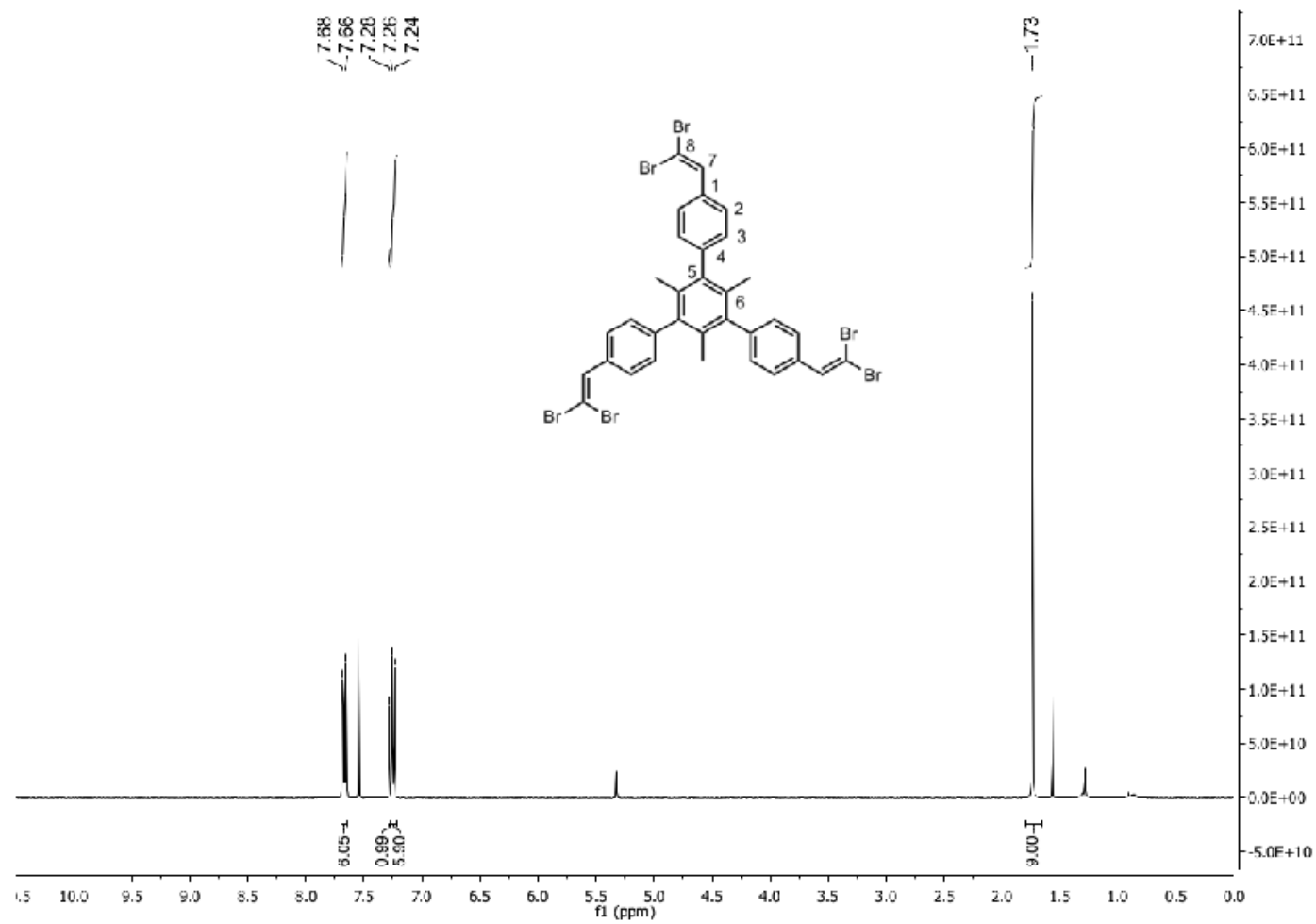


Figure S12 – The ¹³C NMR spectrum of **7**, measured in DMSO-*d*₆.



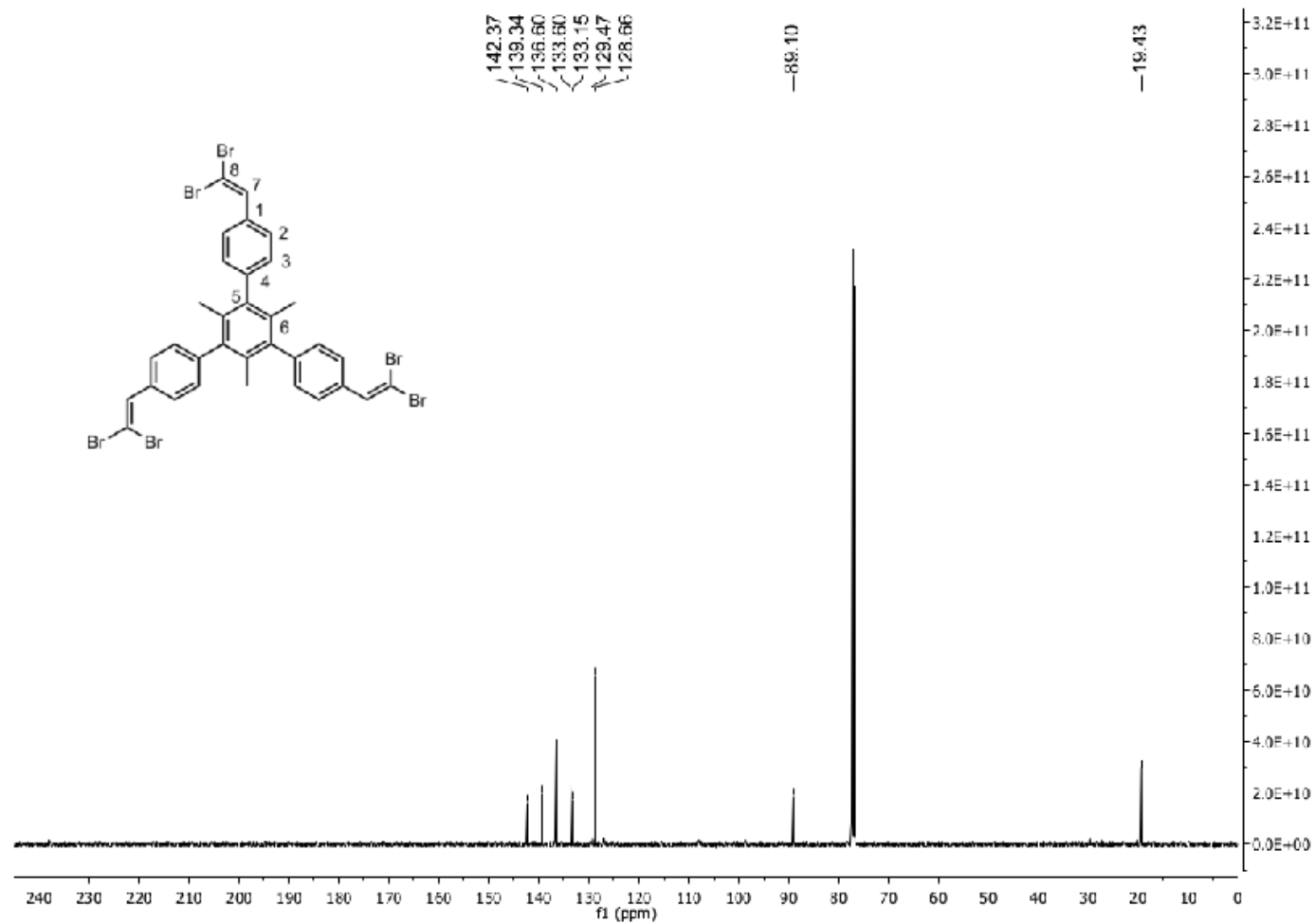


Figure S14 – The ¹³C NMR spectrum of **9**, measured in CDCl₃.

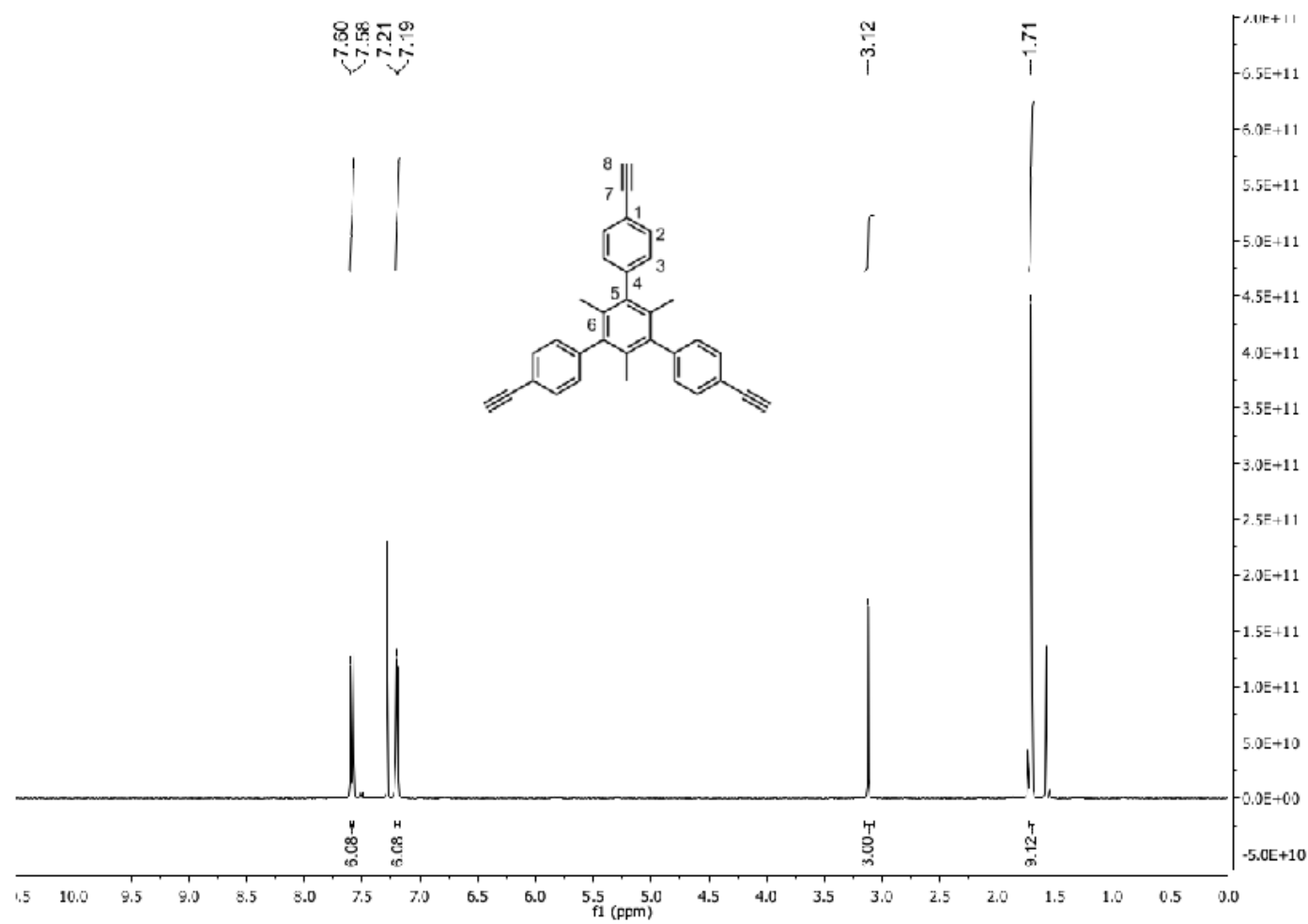


Figure S15 – The ^1H NMR spectrum of **10**, measured in CDCl_3 .

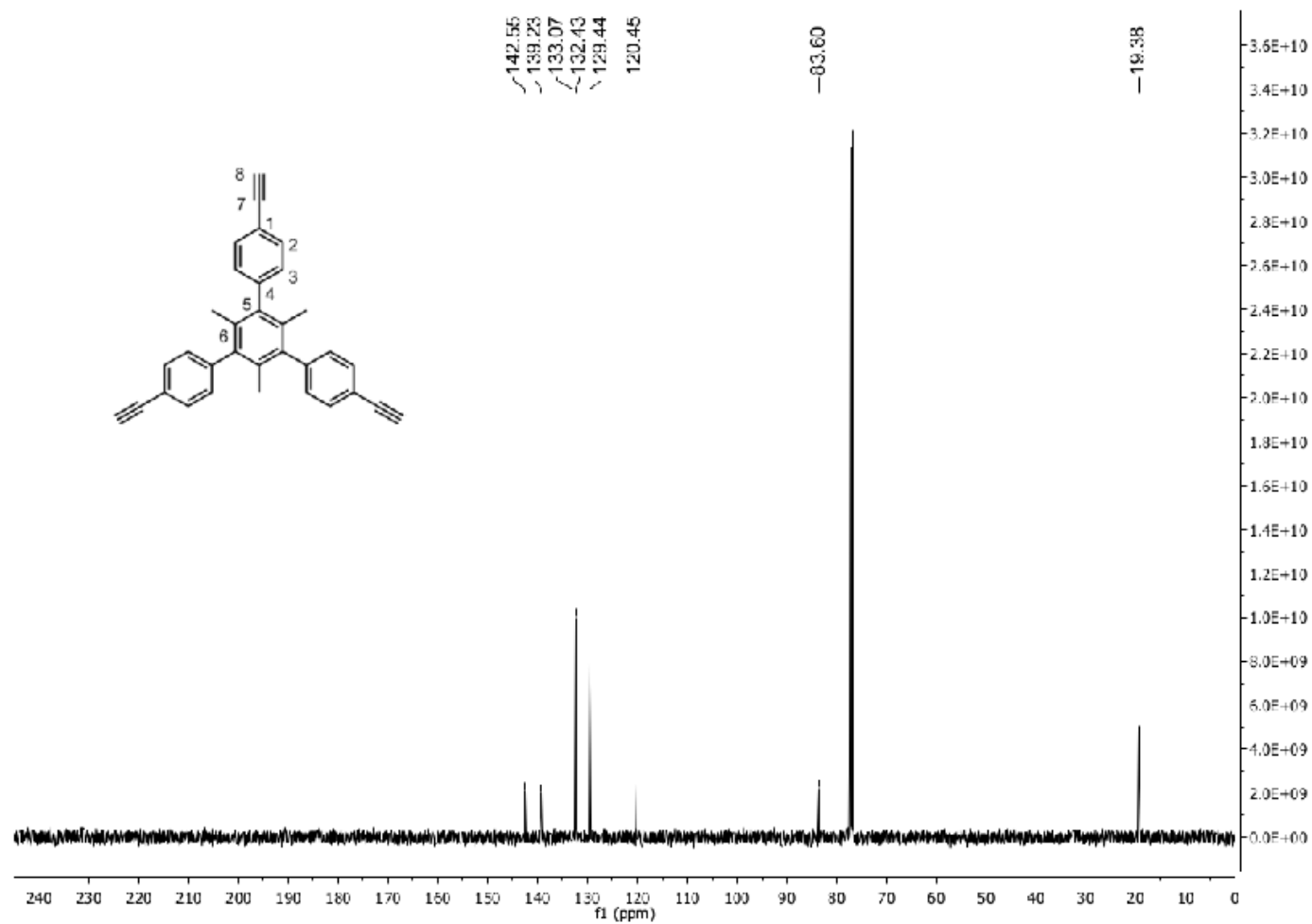


Figure S16 – The ¹³C NMR spectrum of **10**, measured in CDCl₃.

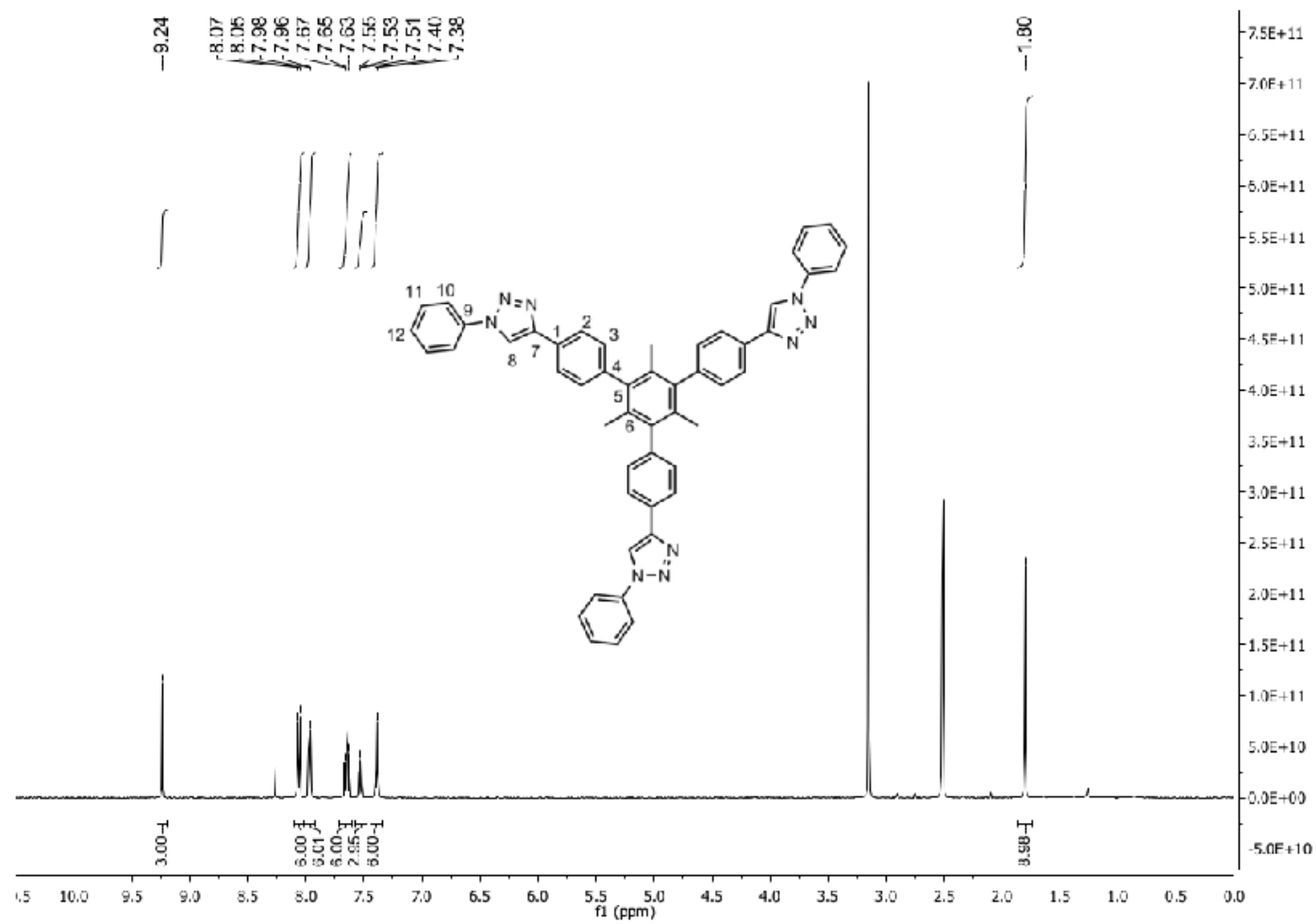


Figure S17 – The ¹H NMR spectrum of **11**, measured in DMSO-*d*₆.

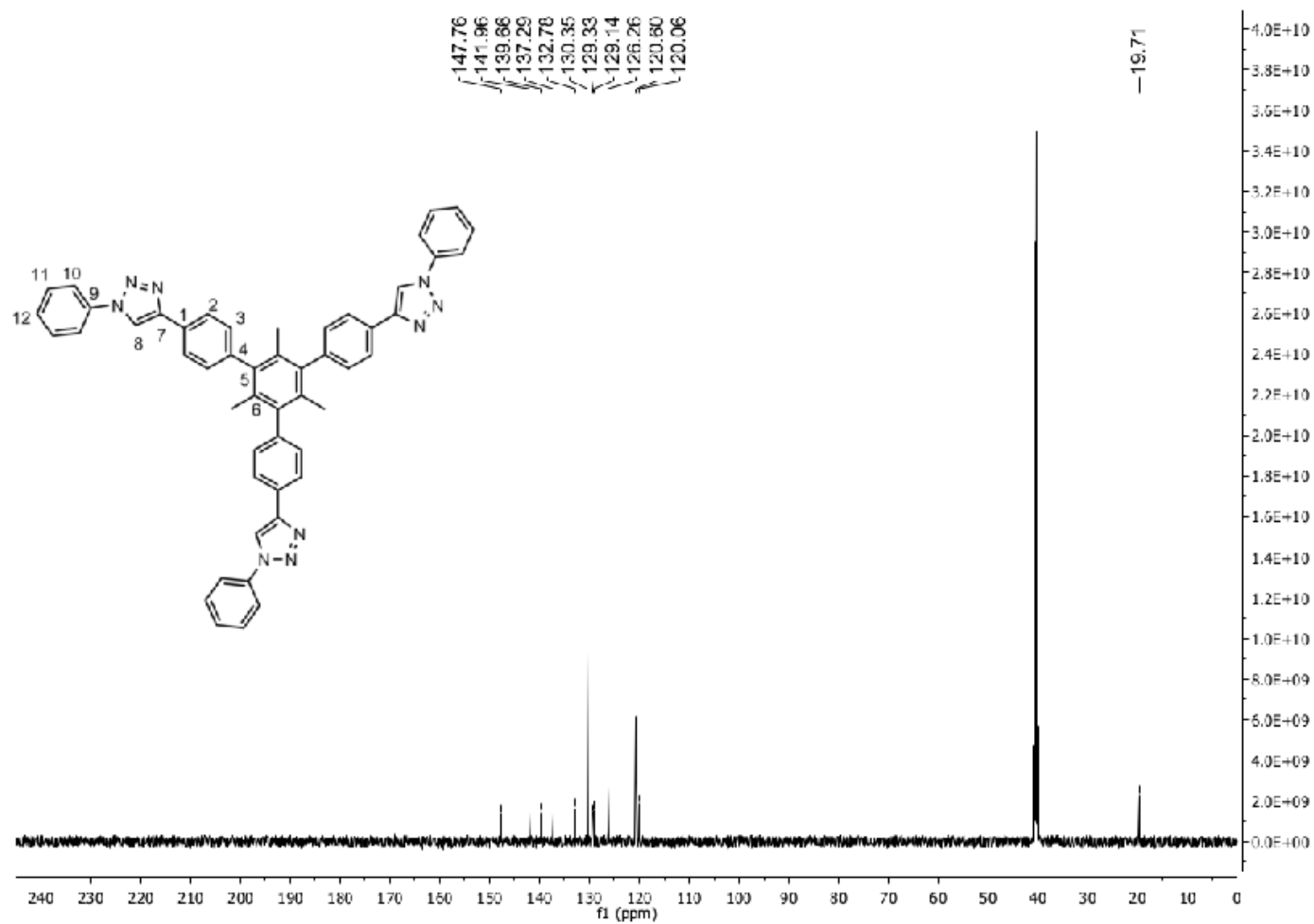


Figure S18 – The ^{13}C NMR spectrum of **11**, measured in $\text{DMSO}-d_6$.

EI-MS Spectra

3CN #996 RT: 3.42 AV: 1 NL: 3.19E7
T: + c EI Full ms [100.00-950.00]

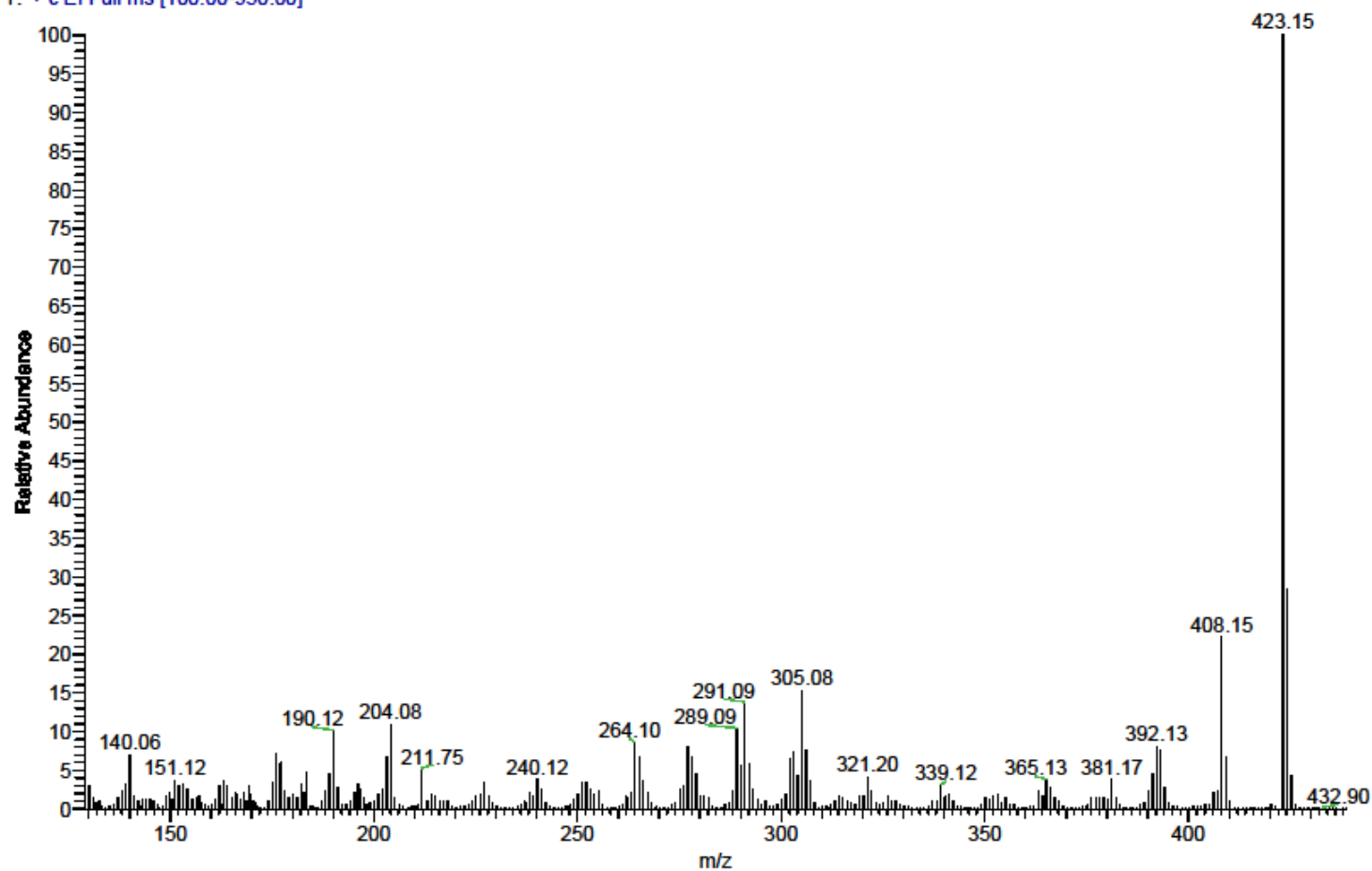


Figure S19 – The EI-MS spectrum of 2.

3TTR #1201 RT: 4.12 AV: 1 NL: 2.27E4
T: + c EI Full ms [100.00-950.00]

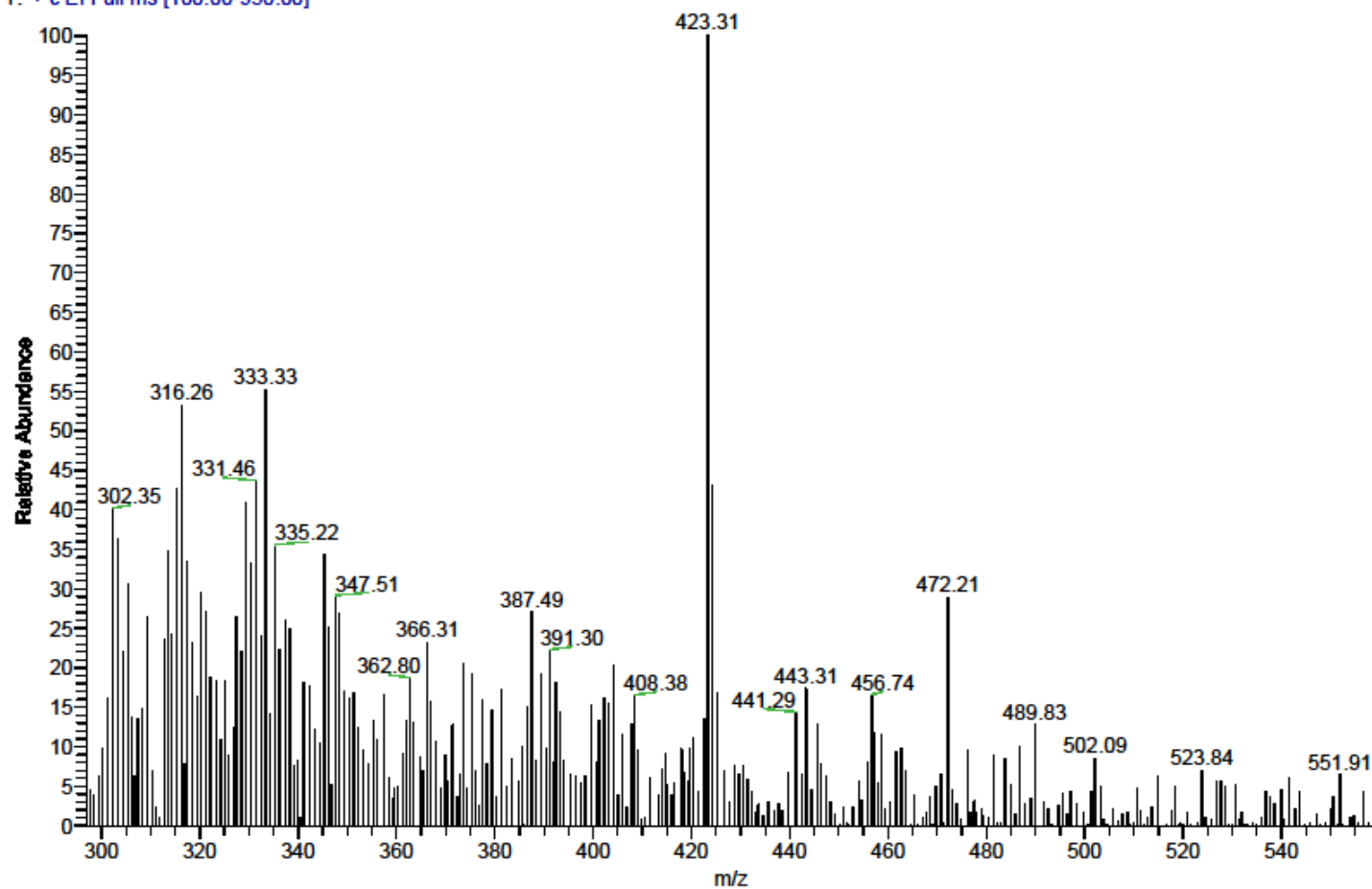


Figure S20 - The EI-MS spectrum of **3**.

3acPhCN #1069-1334 RT: 3.67-4.57 AV: 266 NL: 2.98E5
T: + c EI Full ms [100.00-950.00]

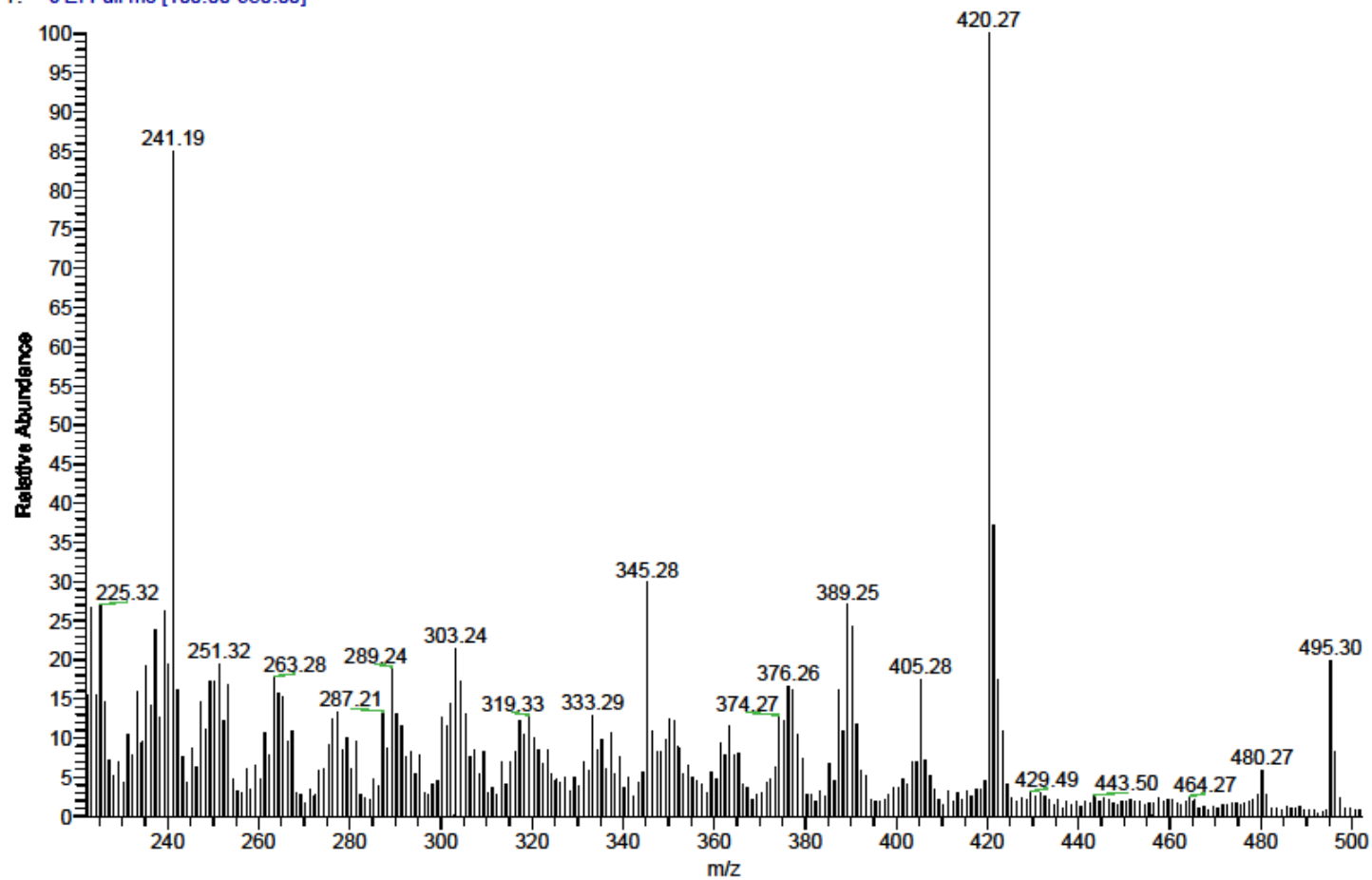


Figure S21 - The EI-MS spectrum of 4.

3acPhCN #1330 RT: 4.55 AV: 1 NL: 1.59E3
T: + c EI Full ms [100.00-950.00]

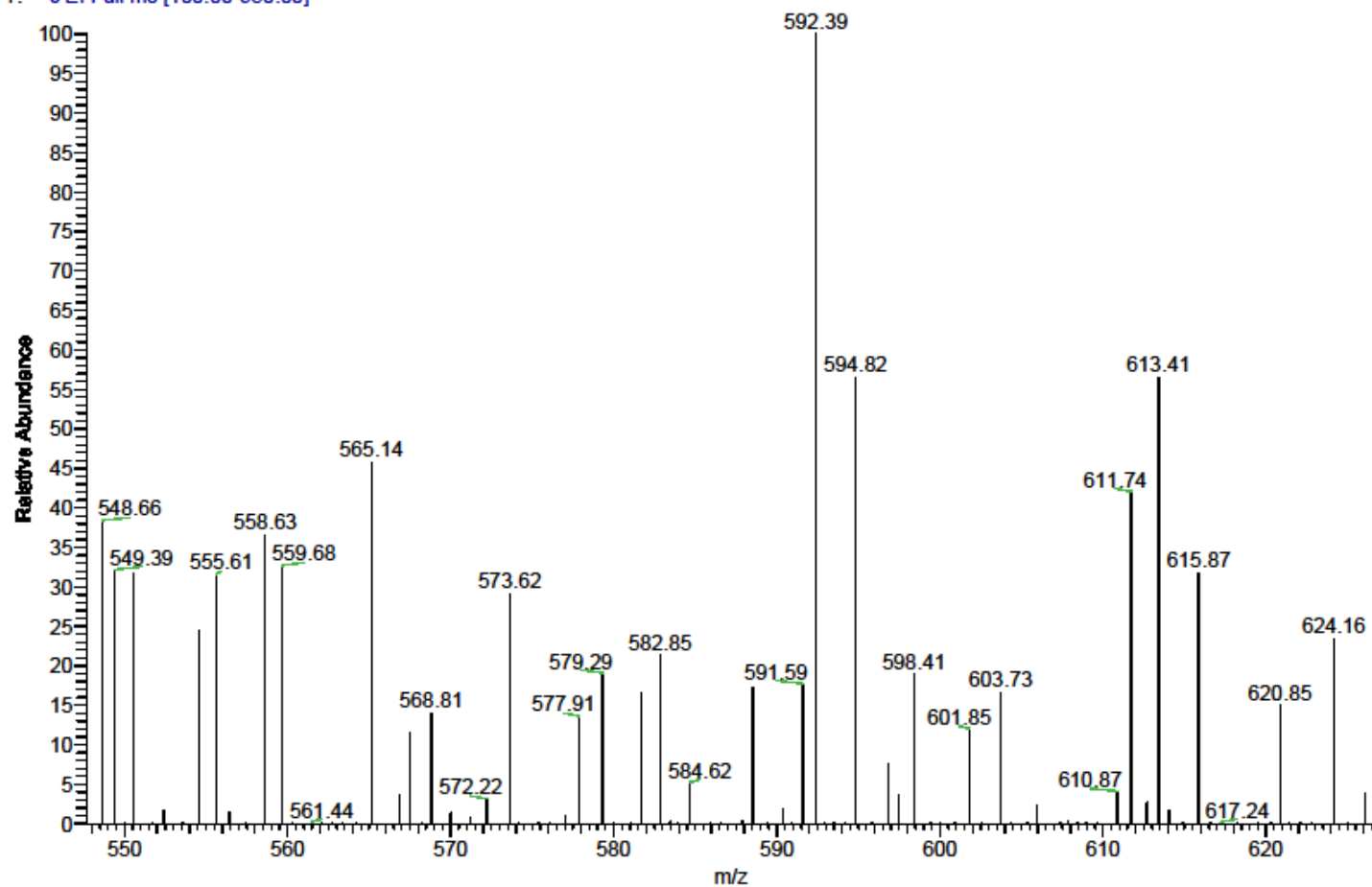


Figure S22 - The EI-MS spectrum of **5**.

3etPhTTR #1192 RT: 4.09 AV: 1 NL: 3.29E5
T: + c EI Full ms [100.00-950.00]

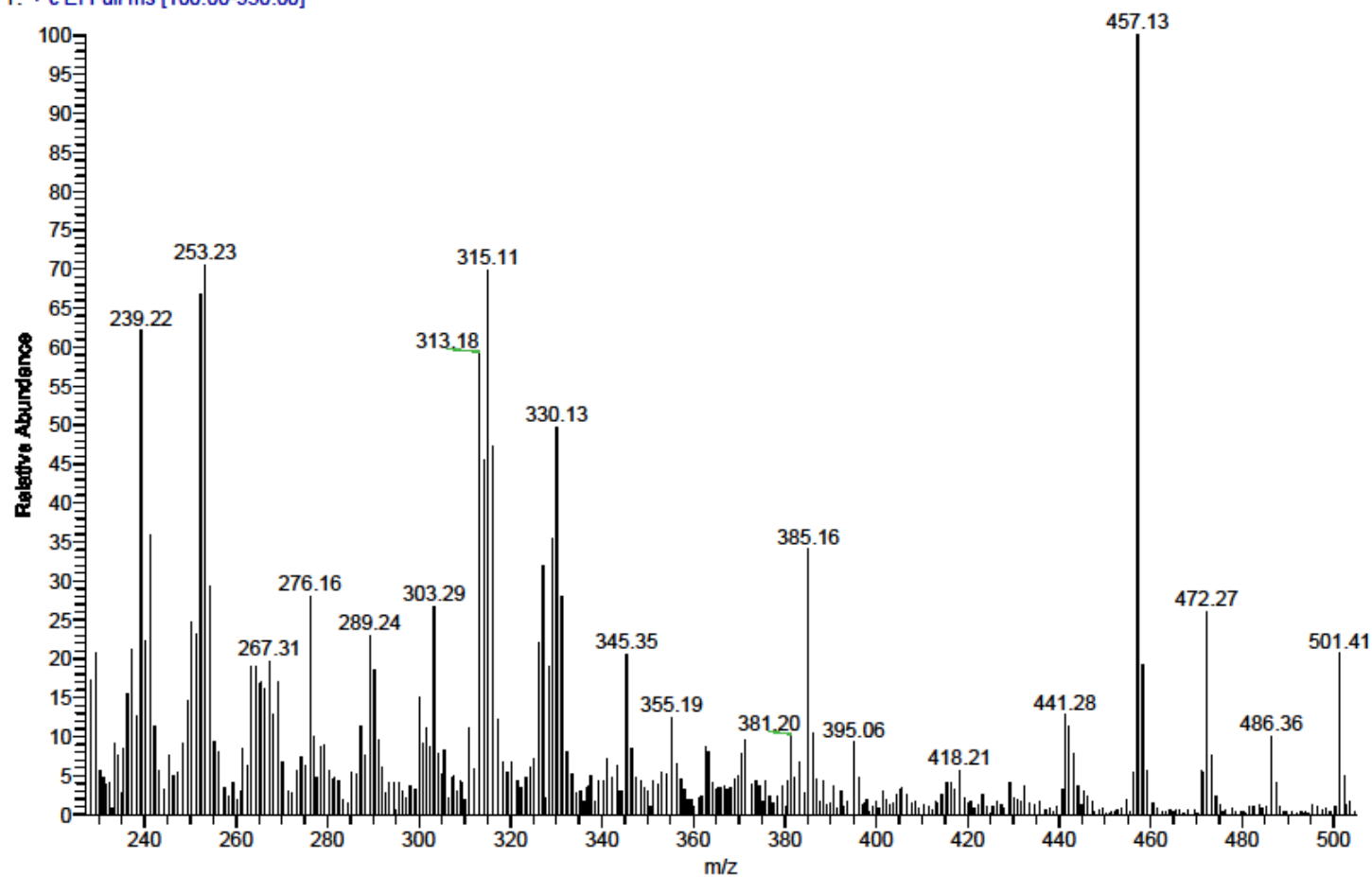


Figure S23 - The EI-MS spectrum of **6**.

3etPhTTR #1269 RT: 4.35 AV: 1 NL: 1.12E4
T: + c EI Full ms [100.00-950.00]

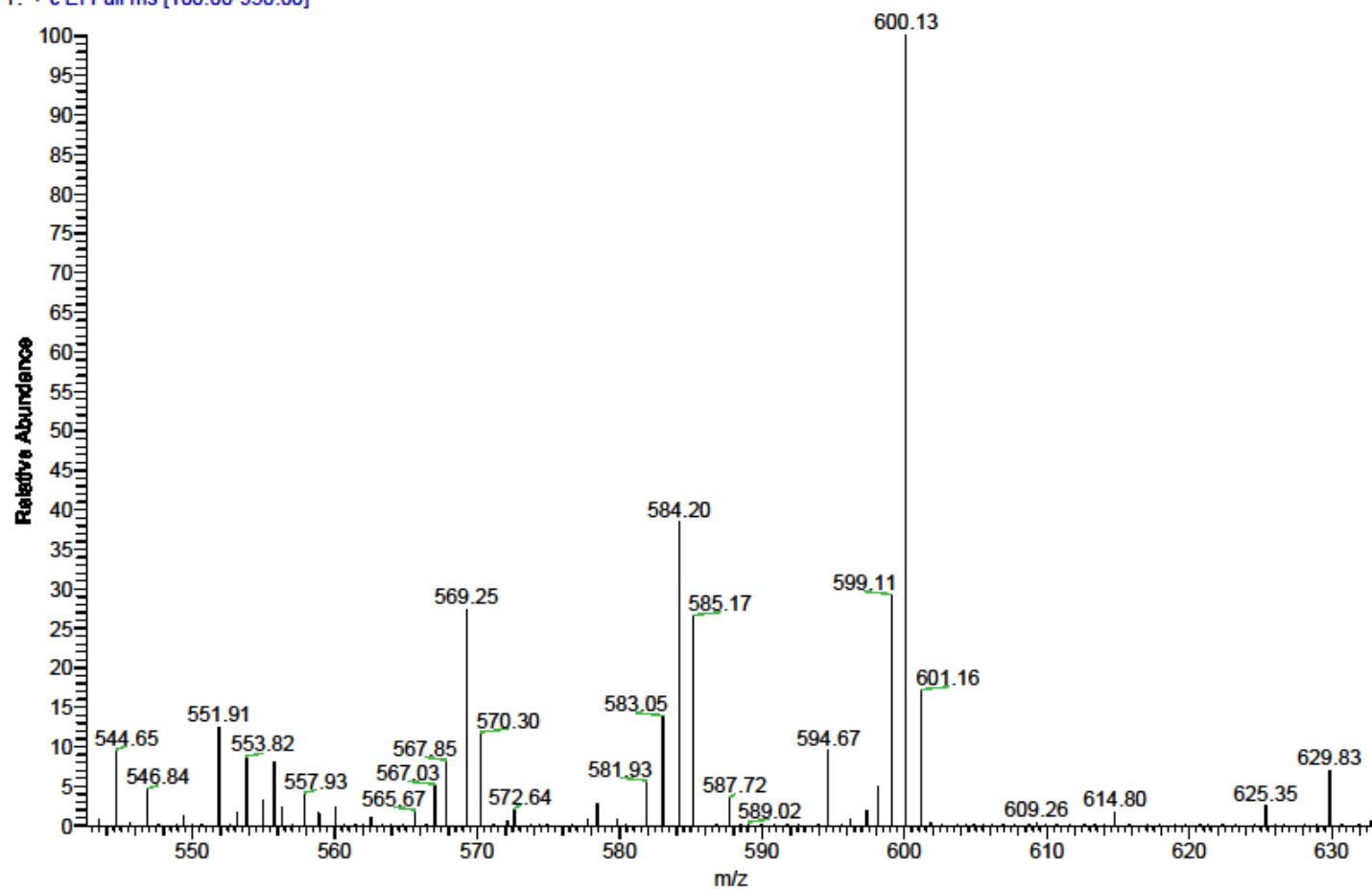


Figure S24 - The EI-MS spectrum of 7.

3CHCBr2_210729124044 #1335 RT: 4.57 AV: 1 NL: 6.81E3
T: + c EI Full ms [100.00-950.00]

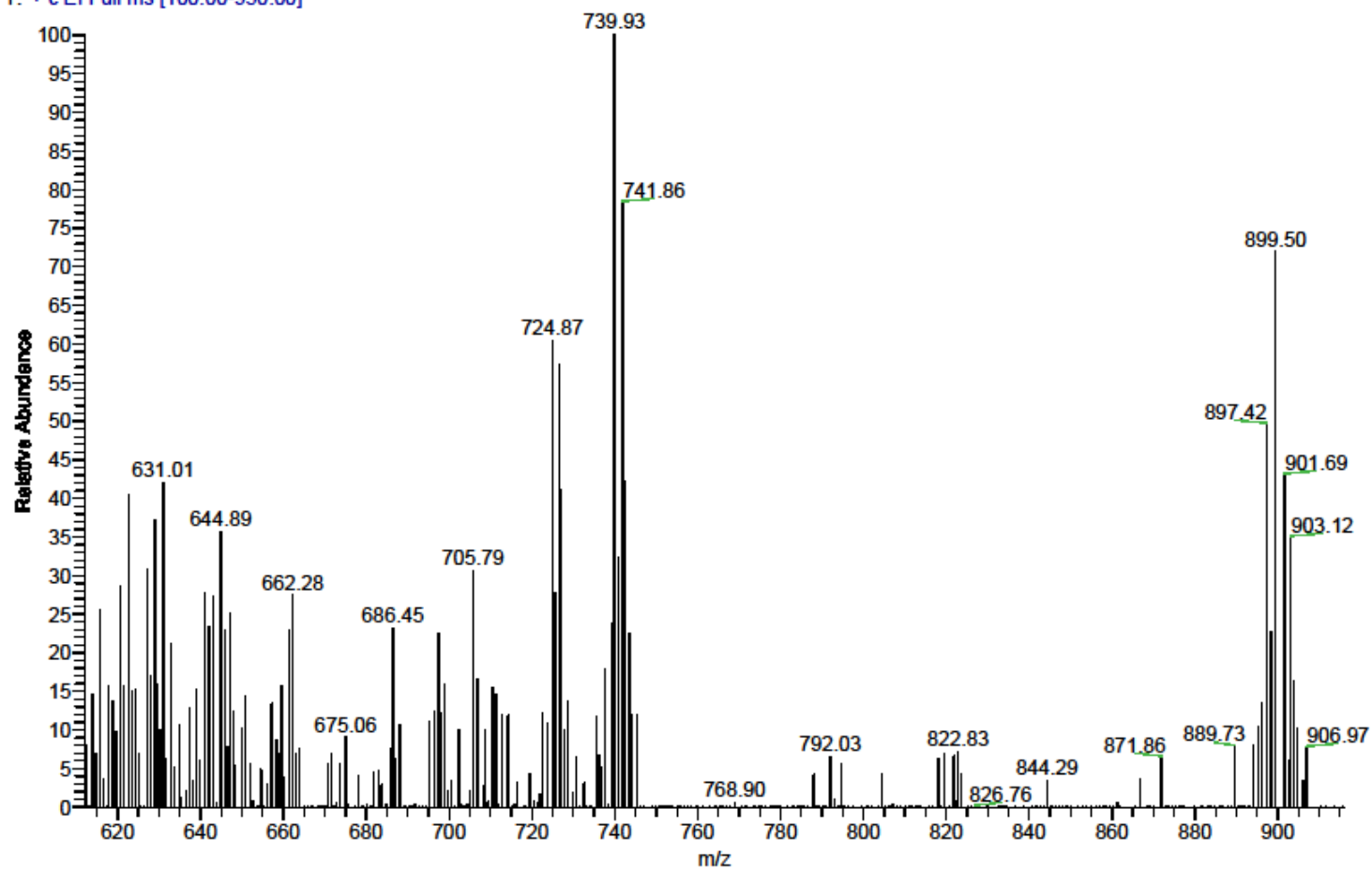


Figure S25 - The EI-MS spectrum of **9**.

3— #1156 RT: 3.96 AV: 1 NL: 1.14E7
T: + c EI Full ms [100.00-950.00]

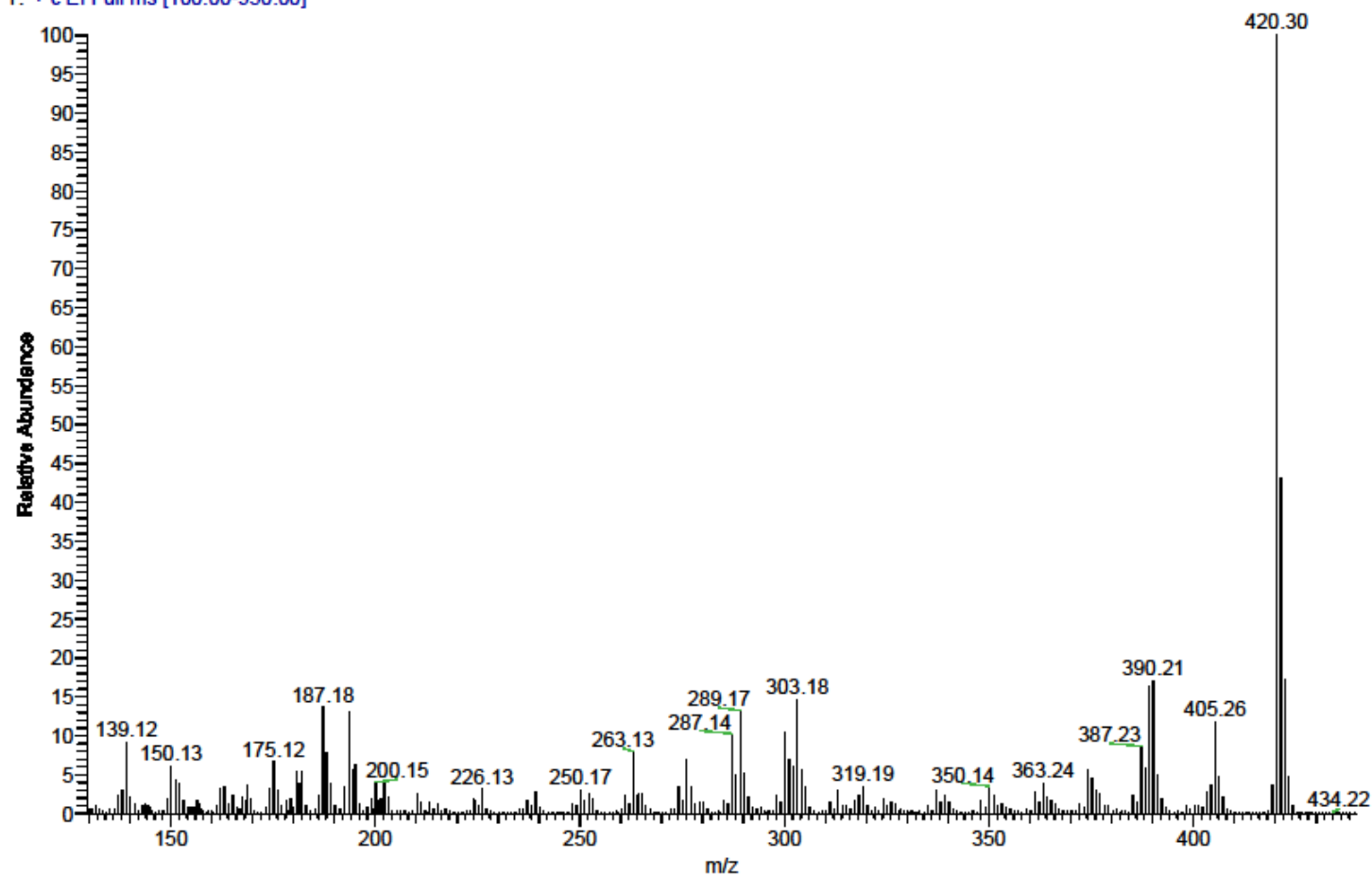


Figure S26 - The EI-MS spectrum of **10**.

3TRZPh #856 RT: 2.94 AV: 1 NL: 1.44E3
T: + c EI Full ms [100.00-950.00]

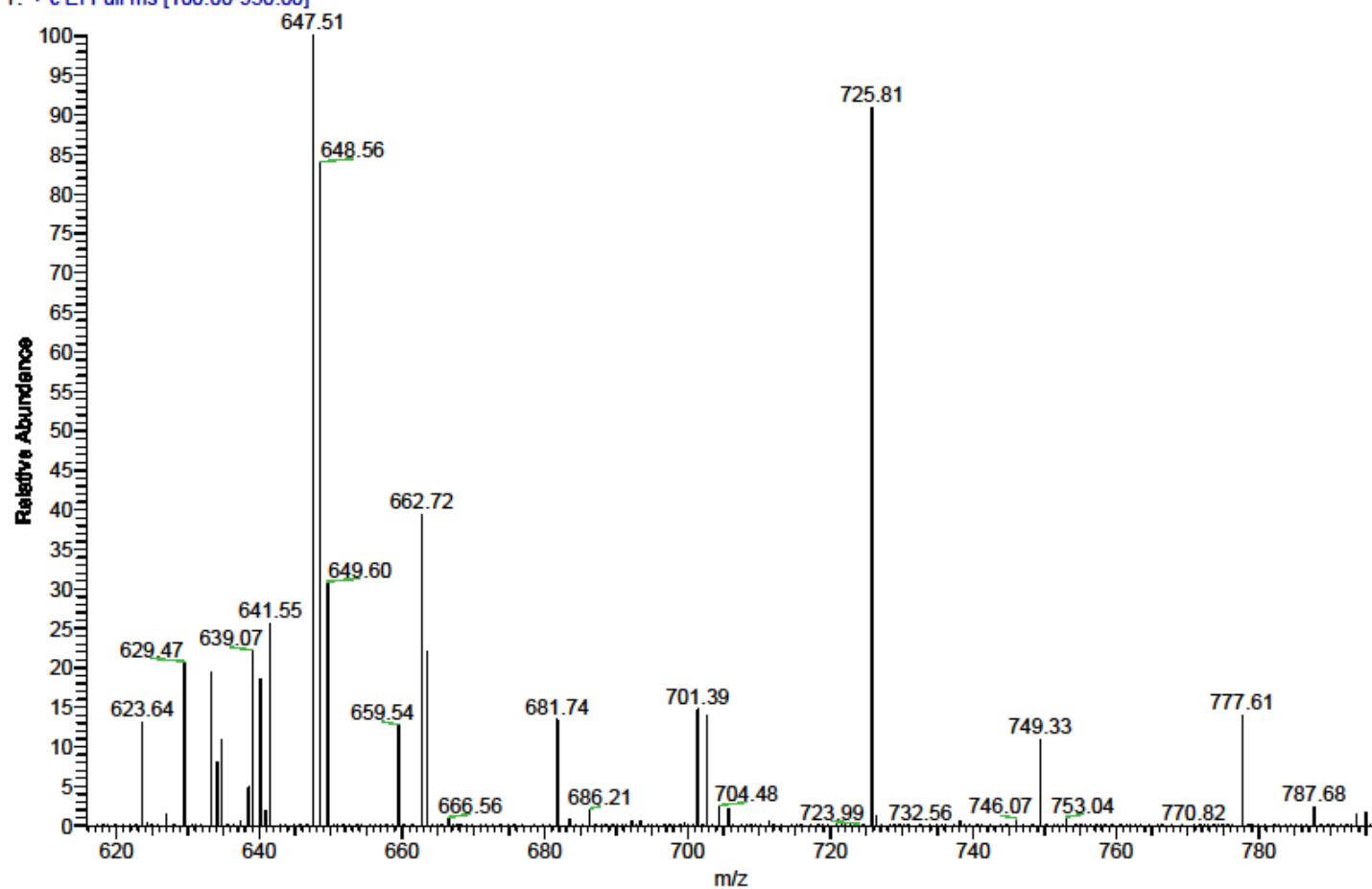


Figure S27 - The EI-MS spectrum of **11**.

X-ray crystallography

Table S1: Crystal data and details of data collection

Parameter	2	9	10	12
empirical formula	C ₃₀ H _{23.25} N ₃ O _{1.13}	C ₃₃ H _{26.75} Br ₆ O _{1.5}	C ₃₃ H ₂₄	C _{55.5} H ₄₆ Ag ₂ F ₆ N ₃ O ₄
<i>F</i> _w	443.76	926.75	420.52	1148.69
space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>C</i> 2/ <i>c</i>
<i>a</i> [Å]	12.0041(12)	20.0818(18)	12.0152(19)	28.8519(7)
<i>b</i> [Å]	8.3857(4)	7.8589(6)	8.6661(15)	18.1939(5)
<i>c</i> [Å]	30.145(3)	21.949(2)	24.388(3)	19.6865(7)
β [°]	122.388(13)	97.147(10)	97.910(14)	96.354(5)
<i>V</i> [Å ³]	2562.5(5)	3437.1(5)	2515.3(7)	10270.5(5)
<i>Z</i>	4	4	4	8
<i>r</i> _{calcd} [g·cm ⁻³]	1.150	1.791	1.110	1.486
Crystal size [mm]	0.20 × 0.05 × 0.05	0.35 × 0.18 × 0.04	0.35 × 0.10 × 0.05	0.45 × 0.30 × 0.03
<i>T</i> [K]	180	297	293	180
μ [mm ⁻¹]	0.071	7.034	0.063	0.832
2 θ range [°]	3.2 to 50.052	5.51 to 50.054	4.462 to 50.054	3.272 to 57.552
Reflections collected	16471	14360	9944	23210
Independent reflections	4503 [<i>R</i> _{int} =0.0450]	6050 [<i>R</i> _{int} =0.1057]	4446 [<i>R</i> _{int} =0.0564]	11697 [<i>R</i> _{int} =0.0356]
Data/restraints/parameter	4503/0/333	6050/0/332	4446/0/301	11697/54/655
<i>R</i> ₁ ^[a]	0.0670	0.0870	0.0764	0.0539
<i>wR</i> ₂ ^[b]	0.1827	0.2768	0.2225	0.1137
GOF ^[c]	1.027	0.999	1.004	1.024
Largest diff. peak/hole / e	0.44/-0.24	1.78/-1.28	0.20/-0.15	0.69/-0.84
CCDC No.	2099115	2099116	2099117	2106774

^a $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$. ^b $wR_2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$. ^c GOF = $\{ \sum [w(F_o^2 - F_c^2)^2] / (n - p) \}^{1/2}$, where *n* is the number of

reflections and *p* is the total number of parameters refined.

Bond distances (Å) and angles(°)

Table S2. Bond distances (Å) for **2**

N1-C1	1.147(4)	C11-C16	1.509(4)
N2-C23	1.144(3)	C12-C13	1.404(3)
N3-C30	1.143(4)	C12-C24	1.498(3)
C1-C2	1.447(4)	C13-C14	1.516(3)
C2-C3	1.384(4)	C17-C18	1.376(4)
C2-C7	1.381(4)	C17-C22	1.377(4)
C3-C4	1.391(4)	C18-C19	1.388(4)
C4-C5	1.394(3)	C19-C20	1.381(4)
C5-C6	1.383(4)	C20-C21	1.365(4)
C5-C8	1.501(3)	C20-C23	1.445(4)
C6-C7	1.379(4)	C21-C22	1.377(4)
C8-C9	1.401(3)	C24-C25	1.390(3)
C8-C13	1.400(3)	C24-C29	1.388(4)
C9-C10	1.402(4)	C25-C26	1.380(4)
C9-C15	1.510(4)	C26-C27	1.381(4)
C10-C11	1.408(3)	C27-C28	1.385(4)
C10-C17	1.502(3)	C27-C30	1.442(4)
C11-C12	1.404(3)	C28-C29	1.381(4)

Table S3. Bond angles(°) for **2**

N1-C1-C2	178.0(3)	C8-C13-C12	119.7(2)
C3-C2-C1	120.4(3)	C8-C13-C14	120.2(2)
C7-C2-C1	119.5(3)	C12-C13-C14	120.1(2)
C7-C2-C3	120.1(2)	C18-C17-C10	122.9(2)
C2-C3-C4	119.7(3)	C18-C17-C22	117.8(2)

C3-C4-C5	120.7(3)	C22-C17-C10	119.3(2)
C4-C5-C8	120.6(2)	C17-C18-C19	120.8(3)
C6-C5-C4	118.1(2)	C20-C19-C18	120.0(3)
C6-C5-C8	121.3(2)	C19-C20-C23	122.0(3)
C7-C6-C5	121.8(2)	C21-C20-C19	119.4(2)
C6-C7-C2	119.6(3)	C21-C20-C23	118.5(2)
C9-C8-C5	120.7(2)	C20-C21-C22	119.9(3)
C13-C8-C5	118.5(2)	C17-C22-C21	121.9(3)
C13-C8-C9	120.8(2)	N2-C23-C20	176.6(3)
C8-C9-C10	118.9(2)	C25-C24-C12	122.0(2)
C8-C9-C15	120.7(2)	C29-C24-C12	120.0(2)
C10-C9-C15	120.4(2)	C29-C24-C25	118.1(2)
C9-C10-C11	121.1(2)	C26-C25-C24	121.4(3)
C9-C10-C17	120.5(2)	C25-C26-C27	119.6(3)
C11-C10-C17	118.2(2)	C26-C27-C28	120.1(2)
C10-C11-C16	120.5(2)	C26-C27-C30	121.0(3)
C12-C11-C10	119.0(2)	C28-C27-C30	118.8(3)
C12-C11-C16	120.6(2)	C29-C28-C27	119.7(3)
C11-C12-C24	120.3(2)	C28-C29-C24	121.1(3)
C13-C12-C11	120.4(2)	N3-C30-C27	178.1(5)
C13-C12-C24	119.3(2)		

Table S4. Bond distances (Å) for **9**

Br1-C1	1.897(10)	C12-C11	1.406(13)
Br2-C1	1.802(13)	C12-C17	1.528(14)
Br3-C25	1.883(12)	C11-C10	1.381(14)
Br4-C25	1.886(13)	C11-C26	1.523(10)
Br5-C33	1.882(13)	C10-C16	1.537(14)
Br6-C33	1.879(10)	C21-C24	1.490(11)

C1-C2	1.305(15)	C21-C20	1.3900
C2-C3	1.489(13)	C21-C22	1.3900
C8-C3	1.3900	C20-C19	1.3900
C8-C7	1.3900	C19-C18	1.3900
C3-C4	1.3900	C18-C23	1.3900
C4-C5	1.3900	C23-C22	1.3900
C5-C6	1.3900	C24-C25	1.307(15)
C6-C7	1.3900	C29-C32	1.460(11)
C6-C9	1.514(10)	C27-C28	1.3900
C9-C14	1.362(13)	C27-C26	1.3900
C9-C10	1.424(14)	C28-C29	1.3900
C14-C13	1.448(14)	C29-C30	1.3900
C14-C15	1.506(14)	C30-C31	1.3900
C13-C12	1.395(14)	C31-C26	1.3900
C13-C18	1.514(11)	C32-C33	1.322(14)

Table S5. Bond angles(°) for **9**

Br2-C1-Br1	111.6(7)	C11-C10-C9	120.5(9)
C2-C1-Br1	120.5(10)	C11-C10-C16	119.5(10)
C2-C1-Br2	127.5(9)	C20-C21-C22	120.0
C1-C2-C3	132.4(11)	C20-C21-C24	115.6(7)
C3-C8-C7	120.0	C22-C21-C24	124.3(7)
C8-C3-C2	124.0(6)	C19-C20-C21	120.0
C4-C3-C2	115.9(6)	C20-C19-C18	120.0
C4-C3-C8	120.0	C19-C18-C13	119.2(6)
C3-C4-C5	120.0	C19-C18-C23	120.0
C4-C5-C6	120.0	C23-C18-C13	120.7(6)
C5-C6-C9	121.9(6)	C18-C23-C22	120.0

C7-C6-C5	120.0	C23-C22-C21	120.0
C7-C6-C9	118.0(6)	C25-C24-C21	133.1(11)
C6-C7-C8	120.0	Br3-C25-Br4	111.9(7)
C14-C9-C6	119.3(8)	C24-C25-Br3	122.0(10)
C14-C9-C10	120.9(9)	C24-C25-Br4	126.1(10)
C10-C9-C6	119.8(8)	C28-C27-C26	120.0
C9-C14-C13	118.7(9)	C29-C28-C27	120.0
C9-C14-C15	122.5(10)	C28-C29-C30	120.0
C13-C14-C15	118.8(9)	C28-C29-C32	115.6(6)
C14-C13-C18	119.0(8)	C30-C29-C32	124.4(6)
C12-C13-C14	120.1(9)	C31-C30-C29	120.0
C12-C13-C18	120.9(9)	C30-C31-C26	120.0
C13-C12-C11	119.9(9)	C27-C26-C11	119.0(6)
C13-C12-C17	119.8(9)	C31-C26-C11	120.5(5)
C11-C12-C17	120.4(9)	C31-C26-C27	120.0
C12-C11-C26	118.8(8)	C33-C32-C29	133.1(10)
C10-C11-C12	119.9(9)	Br6-C33-Br5	112.8(6)
C10-C11-C26	121.3(8)	C32-C33-Br5	124.8(9)
C9-C10-C16	120.0(9)	C32-C33-Br6	122.4(10)

Table S6. Bond distances (Å) for **10**

C1-C2	1.152(5)	C13-C26	1.492(5)
C2-C3	1.446(6)	C14-C15	1.515(5)
C3-C4	1.391(5)	C18-C19	1.369(6)
C3-C8	1.380(6)	C18-C23	1.391(5)
C4-C5	1.379(5)	C19-C20	1.389(6)
C5-C6	1.366(5)	C20-C21	1.379(5)
C6-C7	1.380(5)	C21-C22	1.375(6)
C6-C9	1.501(5)	C21-C24	1.420(6)

C7-C8	1.371(5)	C22-C23	1.383(6)
C9-C10	1.388(5)	C24-C25	1.131(7)
C9-C14	1.400(5)	C26-C27	1.373(5)
C10-C11	1.400(5)	C26-C31	1.383(5)
C10-C16	1.528(5)	C27-C28	1.389(6)
C11-C12	1.408(5)	C28-C29	1.372(6)
C11-C18	1.474(5)	C29-C30	1.372(6)
C12-C13	1.390(5)	C29-C32	1.432(6)
C12-C17	1.515(5)	C30-C31	1.377(5)
C13-C14	1.390(5)	C32-C33	1.145(6)

Table S7. Bond angles(°) for **10**

C1-C2-C3	176.1(6)	C9-C14-C15	120.2(4)
C4-C3-C2	121.0(4)	C13-C14-C9	120.0(4)
C8-C3-C2	120.7(4)	C13-C14-C15	119.8(4)
C8-C3-C4	118.3(4)	C19-C18-C11	121.2(4)
C5-C4-C3	119.1(4)	C19-C18-C23	116.4(5)
C6-C5-C4	122.8(4)	C23-C18-C11	122.3(5)
C5-C6-C7	117.6(4)	C18-C19-C20	122.1(4)
C5-C6-C9	121.5(3)	C21-C20-C19	121.3(5)
C7-C6-C9	120.8(4)	C20-C21-C24	120.6(6)
C8-C7-C6	120.7(4)	C22-C21-C20	116.9(5)
C7-C8-C3	121.4(4)	C22-C21-C24	122.5(5)
C10-C9-C6	119.7(4)	C21-C22-C23	121.8(4)
C10-C9-C14	120.2(4)	C22-C23-C18	121.5(5)
C14-C9-C6	120.1(4)	C25-C24-C21	177.4(8)
C9-C10-C11	120.1(4)	C27-C26-C13	120.2(4)
C9-C10-C16	120.4(4)	C27-C26-C31	117.2(4)
C11-C10-C16	119.5(4)	C31-C26-C13	122.6(4)

C10-C11-C12	119.5(4)	C26-C27-C28	121.9(4)
C10-C11-C18	120.0(4)	C29-C28-C27	120.4(4)
C12-C11-C18	120.5(4)	C28-C29-C32	120.7(5)
C11-C12-C17	119.1(4)	C30-C29-C28	117.9(4)
C13-C12-C11	120.1(4)	C30-C29-C32	121.4(4)
C13-C12-C17	120.8(4)	C29-C30-C31	121.8(4)
C12-C13-C26	119.7(4)	C30-C31-C26	120.8(4)
C14-C13-C12	120.1(4)	C33-C32-C29	177.3(6)
C14-C13-C26	120.1(4)		

Table S8. Bond distances (Å) for **12**

Ag1-O2	2.239(3)	C12-C17	1.401(6)	C41-C43 ⁴	1.352(7)
Ag1-O4	2.289(4)	C13-C14	1.406(5)	C42-C43	1.328(7)
Ag1-N1	2.338(4)	C13-C20	1.511(6)	C44-C45	1.443(9)
Ag1-N3 ¹	2.274(4)	C14-C15	1.398(6)	C45-C46	1.362(9)
Ag2-O1	2.281(3)	C14-C33	1.491(6)	C45-C50	1.388(10)
Ag2-O3	2.219(3)	C15-C16	1.399(6)	C46-C47	1.375(9)
Ag2-N2 ²	2.343(4)	C15-C19	1.514(5)	C47-C48	1.385(11)
F1-C2	1.310(6)	C16-C17	1.405(5)	C48-C49	1.384(13)
F2-C2	1.315(5)	C16-C26	1.500(5)	C49-C50	1.319(10)
F3-C2	1.317(5)	C17-C18	1.509(6)	C51-C52	1.25(2)
F4-C4	1.389(6)	C21-C22	1.367(6)	C52-C53 ⁵	1.398(8)
F5-C4	1.331(7)	C21-C26	1.366(6)	C52-C53	1.403(9)
F6-C4	1.337(6)	C22-C23	1.369(6)	C53-C54	1.392(9)
O1-C1	1.234(5)	C23-C24	1.364(6)	C53-C56 ⁵	1.386(8)
O2-C1	1.230(5)	C23-C27	1.437(6)	C54-C55	1.389(9)
O3-C3	1.234(5)	C24-C25	1.386(6)	C55-C56	1.402(10)
O4-C3	1.234(6)	C25-C26	1.373(6)	C57-C58	1.47(3)
N1-C5	1.142(5)	C28-C29	1.374(7)	C58-C59	1.46(4)

N2-C27	1.145(5)	C28-C33	1.385(7)	C58-C60 ³	1.77(4)
N3-C34	1.126(6)	C29-C30	1.367(7)	C58-C62 ³	0.60(3)
C1-C2	1.535(6)	C30-C31	1.373(6)	C58-C63	1.35(3)
C3-C4	1.475(9)	C30-C34	1.450(6)	C59-C60 ³	0.57(4)
C5-C6	1.432(6)	C31-C32	1.377(6)	C59-C60	1.28(4)
C6-C7	1.376(7)	C32-C33	1.369(6)	C59-C61 ³	1.05(4)
C6-C11	1.388(6)	C35-C36 ³	1.3892(10)	C60-C61	1.39(4)
C7-C8	1.386(6)	C35-C36	1.3891(10)	C61-C62	1.40(3)
C8-C9	1.381(6)	C36-C37	1.3892(10)	C62-C63	1.39(3)
C9-C10	1.374(6)	C37-C38	1.3898(10)	C62-C63 ³	1.39(3)
C9-C12	1.495(6)	C38-C39	1.329(18)	C63-C63 ³	0.000(16)
C10-C11	1.388(6)	C40-C41	1.438(9)		
C12-C13	1.389(6)	C41-C42	1.359(7)		

¹1/2+X,1/2+Y,+Z; ²1/2-X,-1/2+Y,1/2-Z; ³1-X,+Y,1/2-Z; ⁴1/2-X,3/2-Y,-Z; ⁵1/2-X,3/2-Y,1-Z

Table S9. Bond angles(°) for **12**

O2-Ag1-O4	122.83(16)	C13-C14-C33	118.7(4)	C50-C49-C48	121.0(10)
O2-Ag1-N1	116.39(15)	C15-C14-C13	121.0(4)	C49-C50-C45	121.4(8)
O2-Ag1-N3 ¹	115.41(14)	C15-C14-C33	120.3(4)	C51-C52-C53 ⁷	121.8(9)
O4-Ag1-N1	105.20(15)	C14-C15-C16	118.9(4)	C51-C52-C53	125.3(8)
N31-Ag1-O4	96.99(15)	C14-C15-C19	120.7(4)	C537-C52-C53	112.9(14)
N31-Ag1-N1	95.10(15)	C16-C15-C19	120.3(4)	C527-C53-C52	67.1(14)
O1-Ag2-N2 ²	96.30(13)	C15-C16-C17	121.1(4)	C567-C53-C54	171.1(13)
O3-Ag2-O1	147.10(11)	C15-C16-C26	119.7(3)	C55-C54-C53	139.6(16)
O3-Ag2-N2 ²	115.51(13)	C17-C16-C26	119.2(4)	C54-C55-C56	99.4(16)
C1-O1-Ag2	125.4(3)	C12-C17-C16	118.6(4)	C537-C56-C55	128.2(16)
C1-O2-Ag1	124.2(3)	C12-C17-C18	120.3(4)	C57-C58-C60 ⁵	122(2)
C3-O3-Ag2	121.0(3)	C16-C17-C18	121.0(4)	C59-C58-C57	116(2)
C3-O4-Ag1	117.7(3)	C26-C21-C22	122.3(4)	C59-C58-C60 ⁵	17.0(14)

C5-N1-Ag1	146.6(4)	C21-C22-C23	119.5(5)	C625-C58-C57	42(5)
C27-N2-Ag2 ³	152.8(4)	C22-C23-C27	120.8(4)	C625-C58-C59	157(6)
C34-N3-Ag1 ⁴	168.0(4)	C24-C23-C22	119.6(4)	C625-C58-C60 ⁵	153(6)
O1-C1-C2	116.8(4)	C24-C23-C27	119.6(4)	C625-C58-C63	81(5)
O2-C1-O1	129.9(4)	C23-C24-C25	120.2(4)	C63-C58-C57	122.4(19)
O2-C1-C2	113.2(4)	C26-C25-C24	120.7(5)	C63-C58-C59	122(2)
F1-C2-F2	107.6(4)	C21-C26-C16	122.0(4)	C63-C58-C60 ⁵	113(2)
F1-C2-F3	106.6(5)	C21-C26-C25	117.7(4)	C60-C59-C58	110(3)
F1-C2-C1	113.6(4)	C25-C26-C16	120.3(4)	C605-C59-C58	114(7)
F2-C2-F3	106.5(4)	N2-C27-C23	178.4(5)	C605-C59-C60	60(7)
F2-C2-C1	111.6(4)	C29-C28-C33	121.0(5)	C605-C59-C61 ⁵	115(7)
F3-C2-C1	110.5(4)	C30-C29-C28	120.0(5)	C615-C59-C58	47(2)
O3-C3-C4	115.2(5)	C29-C30-C31	120.2(4)	C615-C59-C60	155(4)
O4-C3-O3	130.4(5)	C29-C30-C34	118.9(4)	C59-C60-C61	134(4)
O4-C3-C4	114.4(5)	C31-C30-C34	120.9(4)	C585-C61-C57 ⁵	66.7(19)
F4-C4-C3	110.2(6)	C30-C31-C32	119.1(4)	C585-C61-C60	91(3)
F5-C4-F4	102.0(6)	C33-C32-C31	122.0(4)	C585-C61-C62	23.7(18)
F5-C4-F6	111.5(8)	C28-C33-C14	120.1(4)	C60-C61-C57 ⁵	156(2)
F5-C4-C3	112.9(6)	C32-C33-C14	122.1(4)	C60-C61-C62	113(2)
F6-C4-F4	101.3(6)	C32-C33-C28	117.7(4)	C62-C61-C57 ⁵	44.2(13)
F6-C4-C3	117.1(5)	N3-C34-C30	177.1(5)	C575-C62-C61	73.4(18)
N1-C5-C6	178.2(5)	C36-C35-C36 ⁵	107.3(12)	C575-C62-C63 ⁵	166(3)
C7-C6-C5	119.9(4)	C35-C36-C37	129.9(10)	C575-C62-C63	166(3)
C7-C6-C11	120.1(4)	C36-C37-C38	116.0(8)	C635-C62-C61	118(2)
C11-C6-C5	120.0(4)	C375-C38-C37	120.5(10)	C63-C62-C61	118(2)
C6-C7-C8	120.3(5)	C39-C38-C37	119.7(5)	C635-C62-C63	0.0(6)
C9-C8-C7	120.2(5)	C39-C38-C37 ⁵	119.7(5)	C58-C63-C58 ⁵	97(2)
C8-C9-C12	119.7(4)	C42-C41-C40	116.3(10)	C58-C63-C62	122.0(16)
C10-C9-C8	119.1(4)	C436-C41-C40	120.2(9)	C585-C63-C62	25.4(11)
C10-C9-C12	121.2(4)	C436-C41-C42	123.4(7)	C58-C63-C62 ⁵	25.4(11)
C9-C10-C11	121.4(4)	C43-C42-C41	116.8(7)	C585-C63-C62 ⁵	122.0(16)
C10-C11-C6	118.9(5)	C42-C43-C41 ⁶	119.8(7)	C625-C63-C62	147(2)
C13-C12-C9	119.5(4)	C46-C45-C44	122.2(8)	C635-C63-C58 ⁵	0(10)
C13-C12-C17	121.4(4)	C46-C45-C50	118.2(7)	C635-C63-C58	0(10)

C17-C12-C9	119.1(4)	C50-C45-C44	119.6(8)	C635-C63-C62	0(10)
C12-C13-C14	119.0(4)	C45-C46-C47	121.5(7)	C635-C63-C62 ⁵	0(10)
C12-C13-C20	119.8(4)	C46-C47-C48	118.9(8)		
C14-C13-C20	121.2(4)	C49-C48-C47	119.0(8)		

¹1/2+X,1/2+Y,+Z; ²1/2-X,-1/2+Y,1/2-Z; ³1/2-X,1/2+Y,1/2-Z; ⁴-1/2+X,-1/2+Y,+Z; ⁵1-X,+Y,1/2-Z; ⁶1/2-X,3/2-Y,-Z; ⁷1/2-X,3/2-Y,1-Z