Electronic supporting information

Extended tetrathiafulvalene with a pentaleno[1,2-*b*:4,5-*b*']difluorene core – A donor-acceptor multi-redox system

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Characterization data

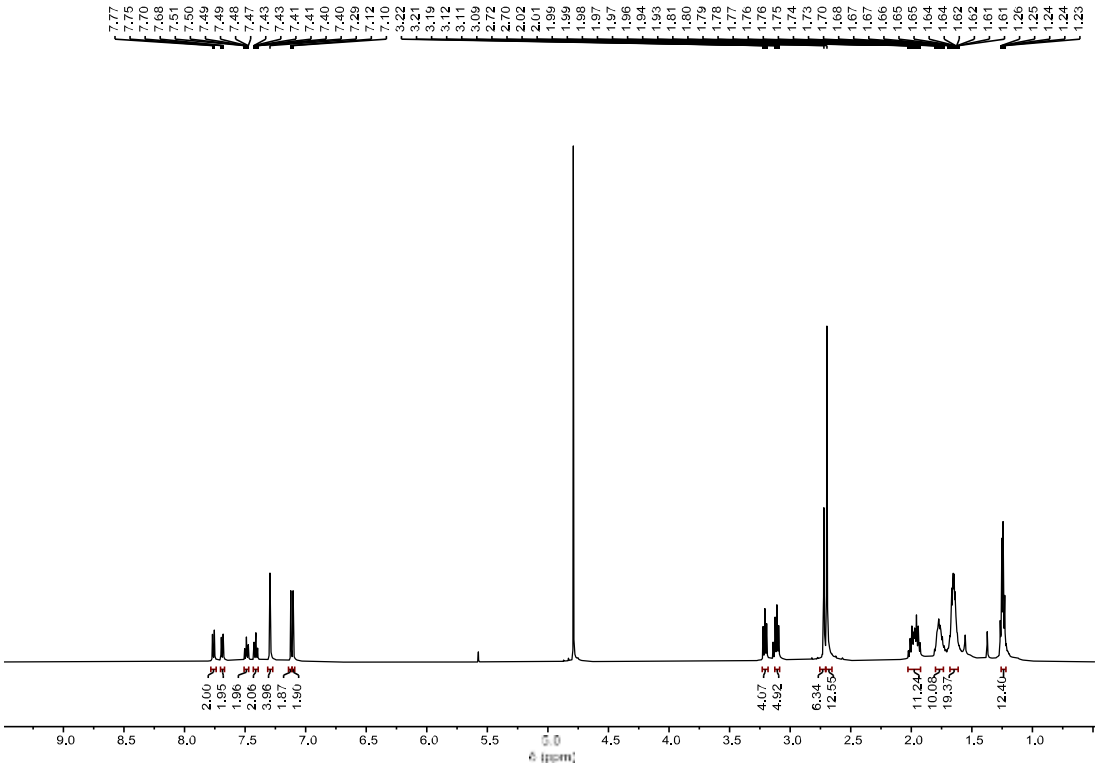


Figure S1 – ^{1}H NMR (CS_2 (D_2O log tube), 500 MHz) spectrum of **G**.

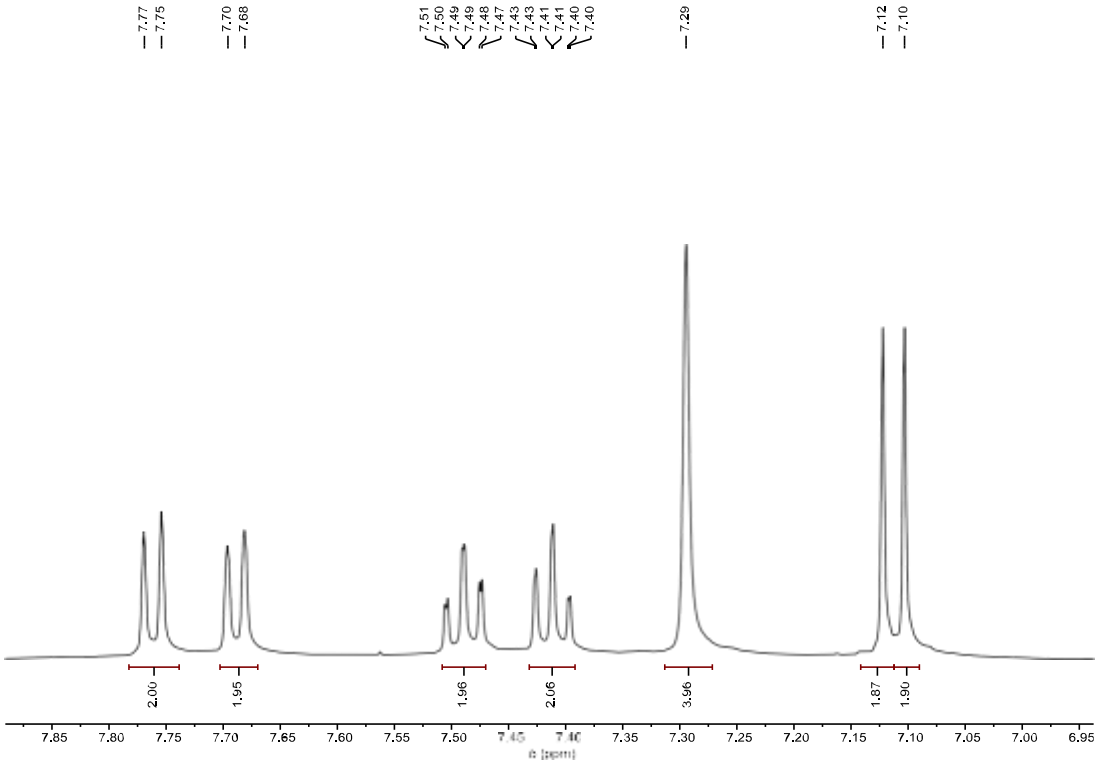


Figure S2 – ^{1}H NMR (CS_2 (D_2O log tube), 500 MHz) spectrum of **G** – Selected region.

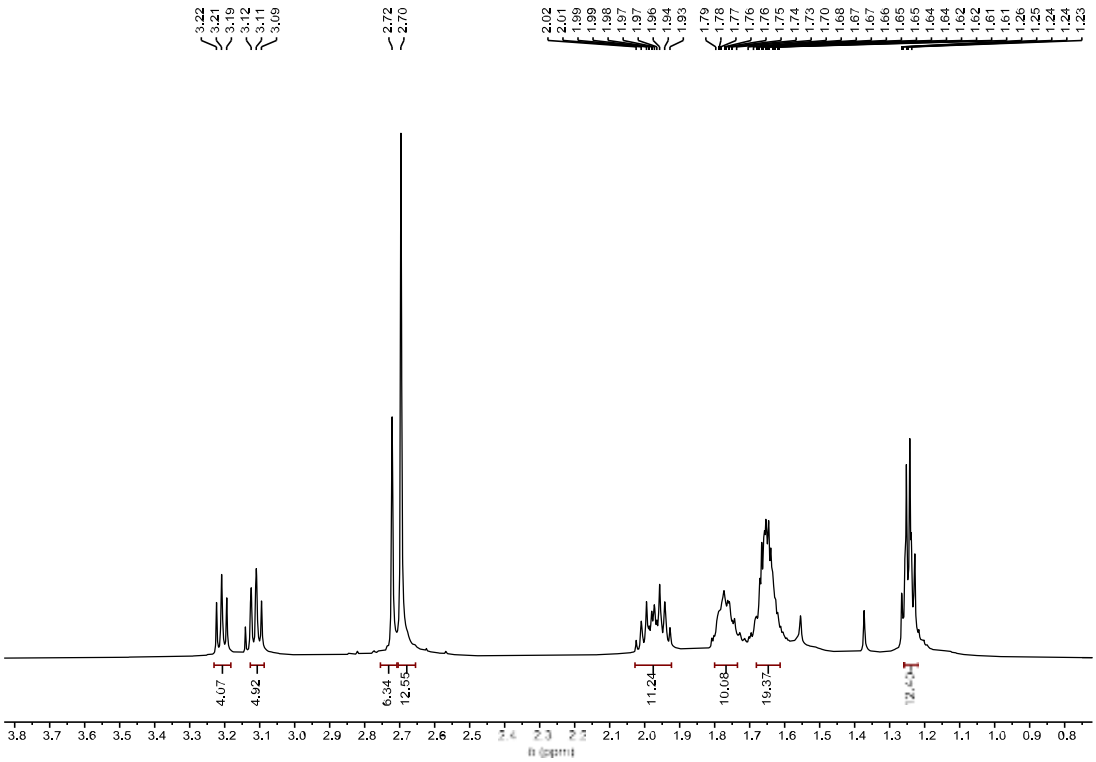


Figure S3 – ^{1}H NMR (CS_2 (D_2O log tube), 500 MHz) spectrum of **G** – Selected region.

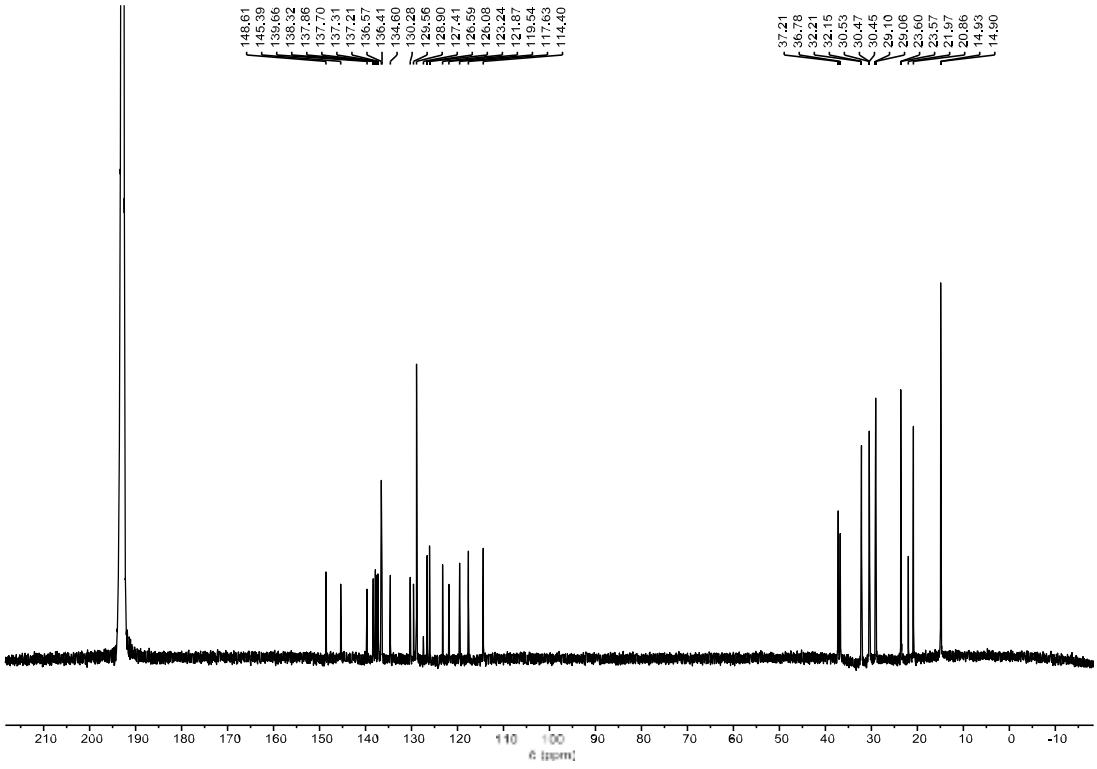


Figure S4 – ^{13}C NMR (CS_2 (D_2O log tube), 126 MHz) spectrum of **G**.

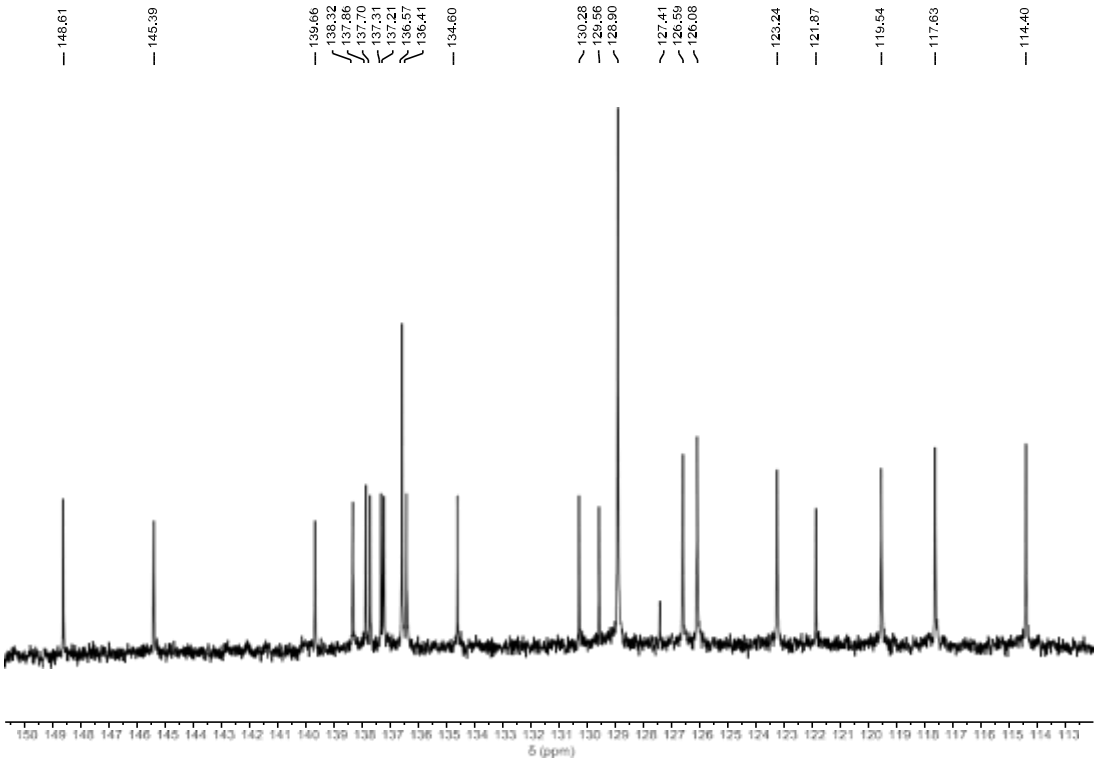


Figure S5 – ^{13}C NMR (CS_2 (D_2O log tube), 126 MHz) spectrum of **G** – Selected region.

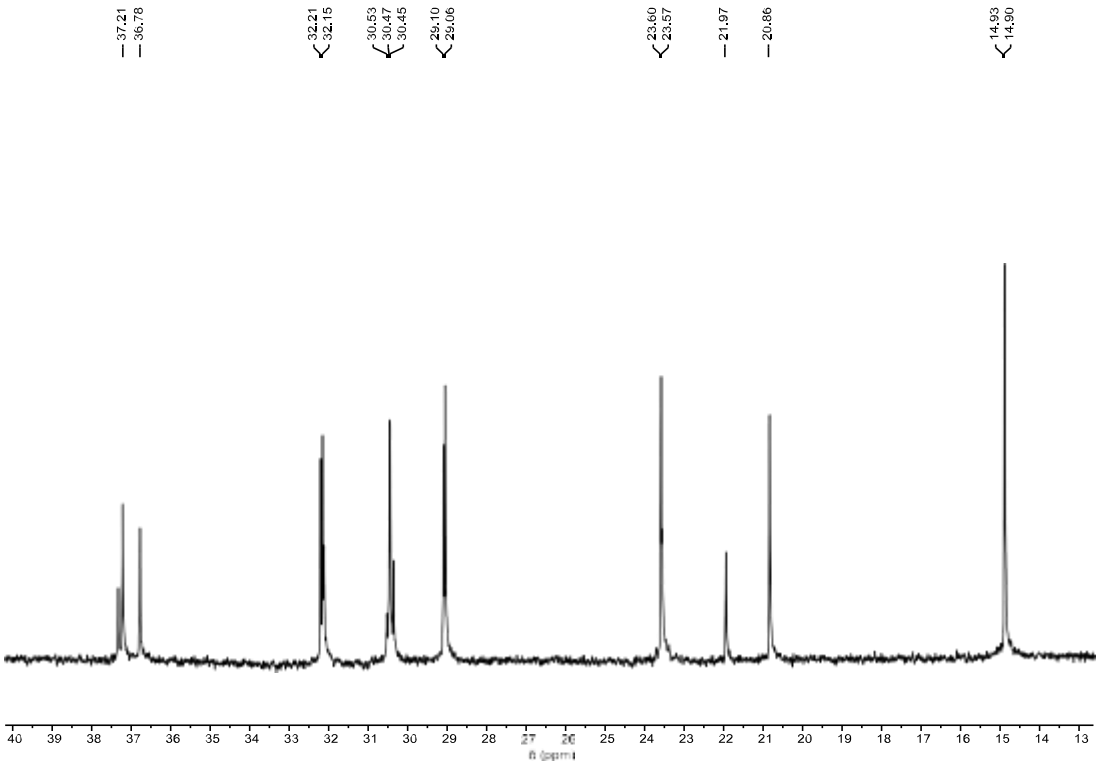


Figure S6 – ^{13}C NMR (CS_2 (D_2O log tube), 126 MHz) spectrum of **G** – Selected region.

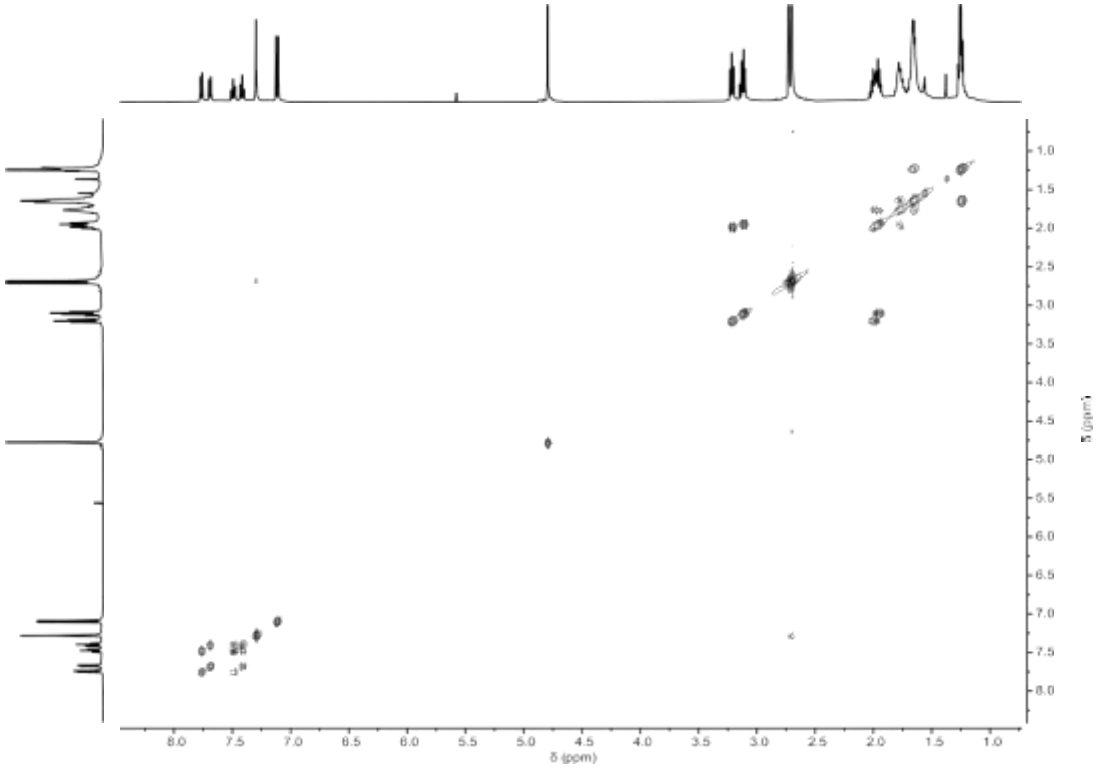


Figure S7 – $^{1}H/^{1}H$ COSY (CS_2 (D_2O log tube), 500/500 MHz) spectrum of **G.**

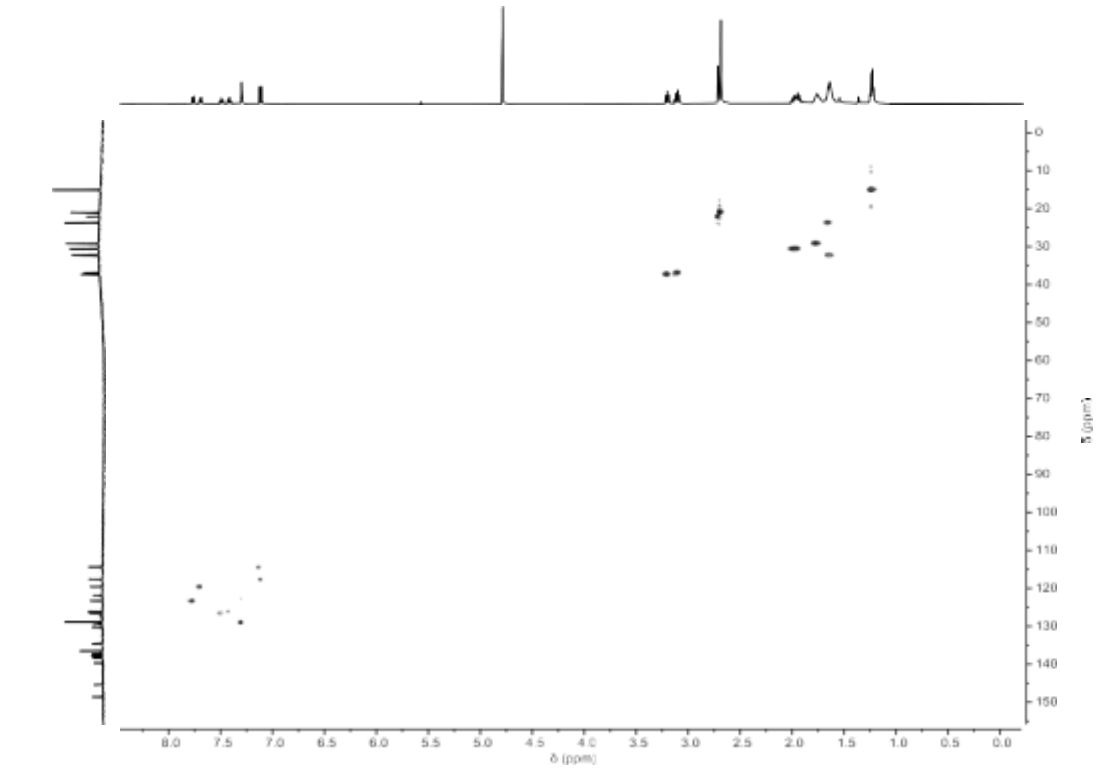


Figure S8 – $^{1}H/^{13}C$ HSQC (CS_2 (D_2O log tube), 500/126 MHz) spectrum of **G**.

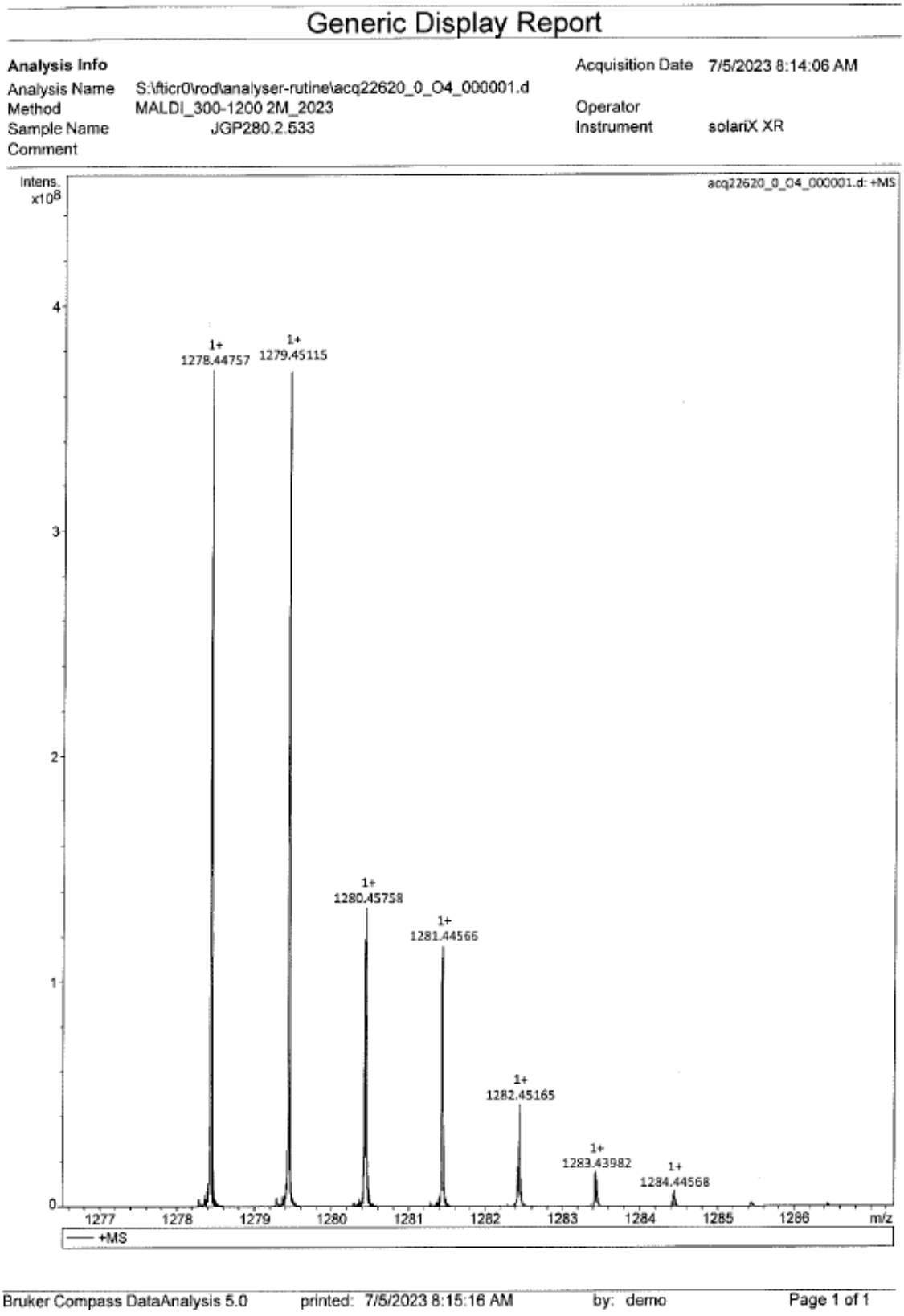


Figure SG - HRMS (MALDI$^+$, dithranol) spectrum of **G**.

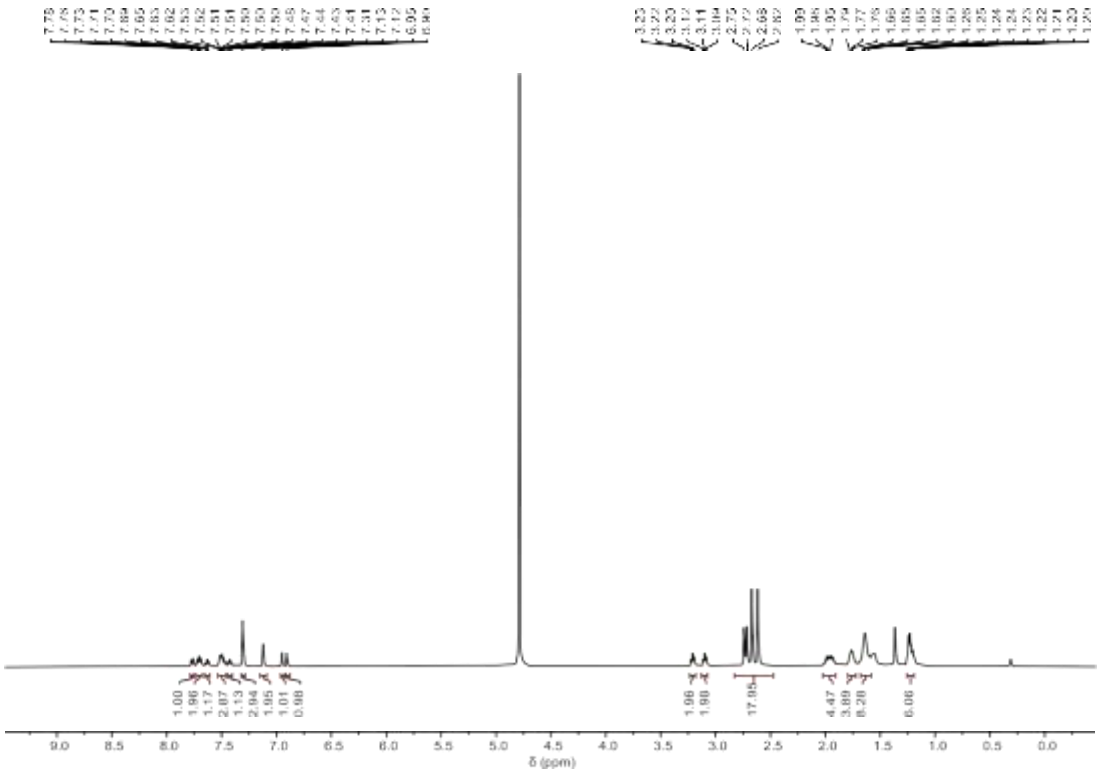


Figure S10 – ^{1}H NMR (CS_2 (D_2O log tube), 500 MHz) spectrum of **10**.

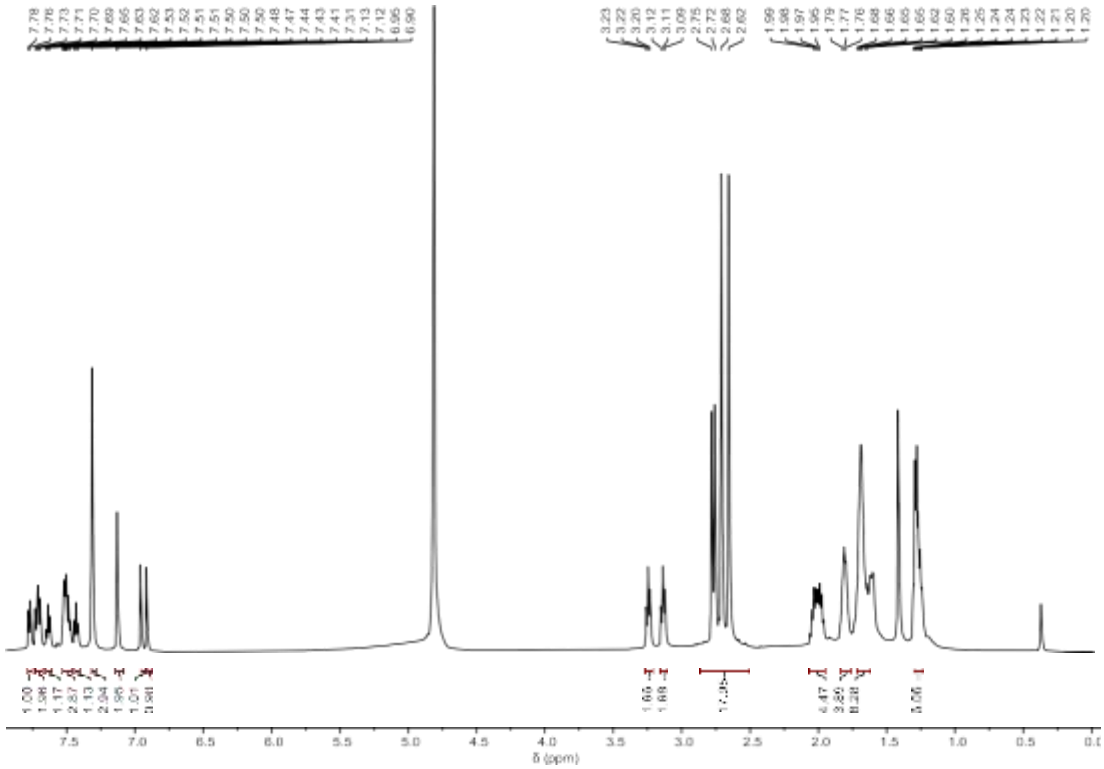


Figure S11 – ^{1}H NMR (CS_2 (D_2O log tube), 500 MHz) spectrum of **10** – Selected region.

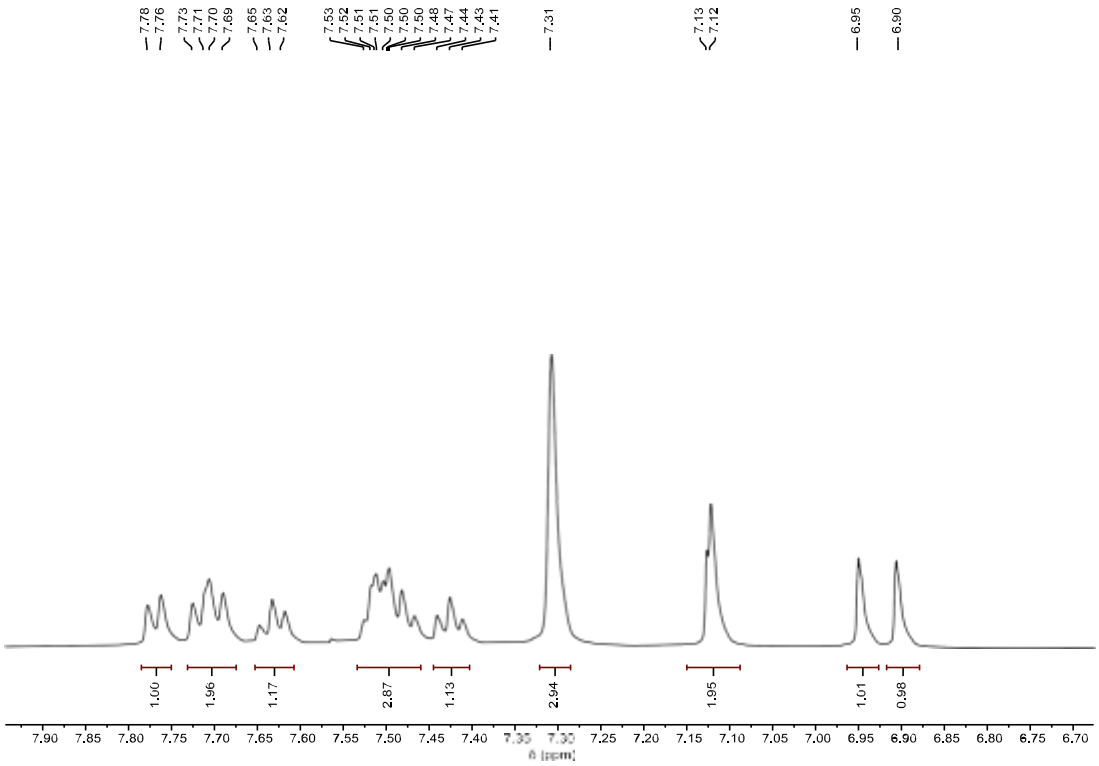


Figure S12 – ^{1}H NMR (CS_2 (D_2O log tube), 500 MHz) spectrum of **10** – Selected region.

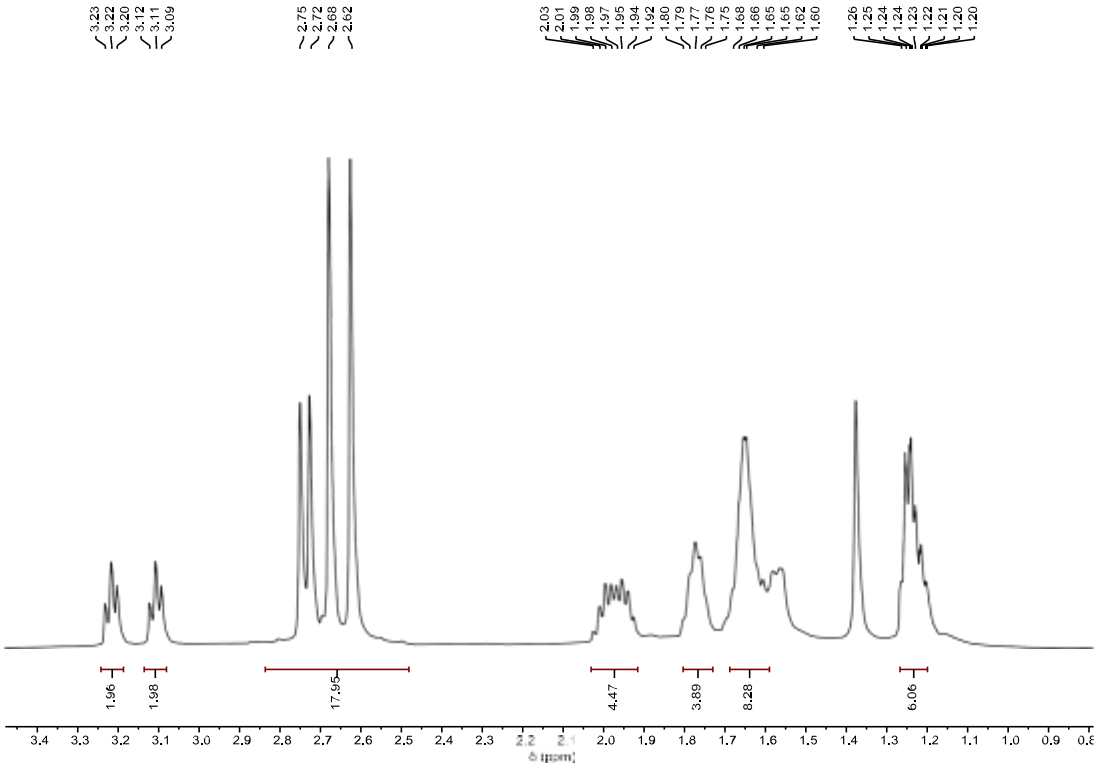


Figure S13 – ^{1}H NMR (CS_2 (D_2O log tube), 500 MHz) spectrum of **10** – Selected region.

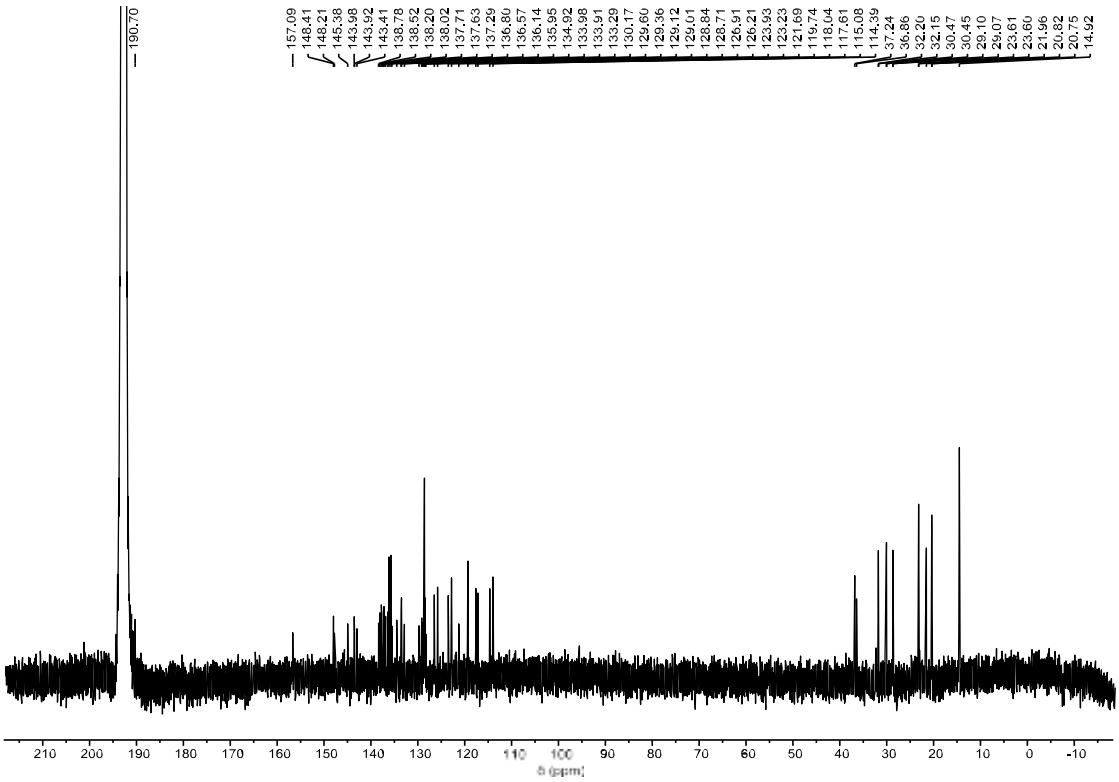


Figure S14 – ^{13}C NMR (CS_2 (D_2O log tube), 126 MHz) spectrum of **10**.

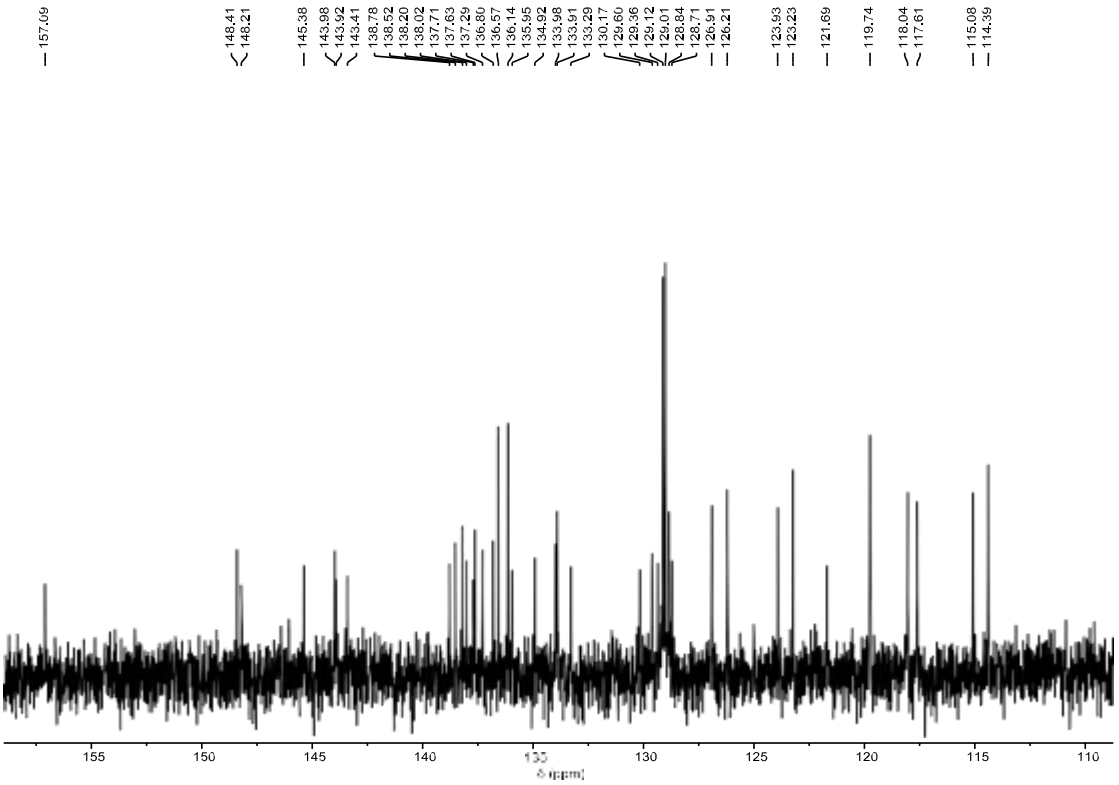


Figure S15 – ^{13}C NMR (CS_2 (D_2O log tube), 126 MHz) spectrum of **10** – Selected region.

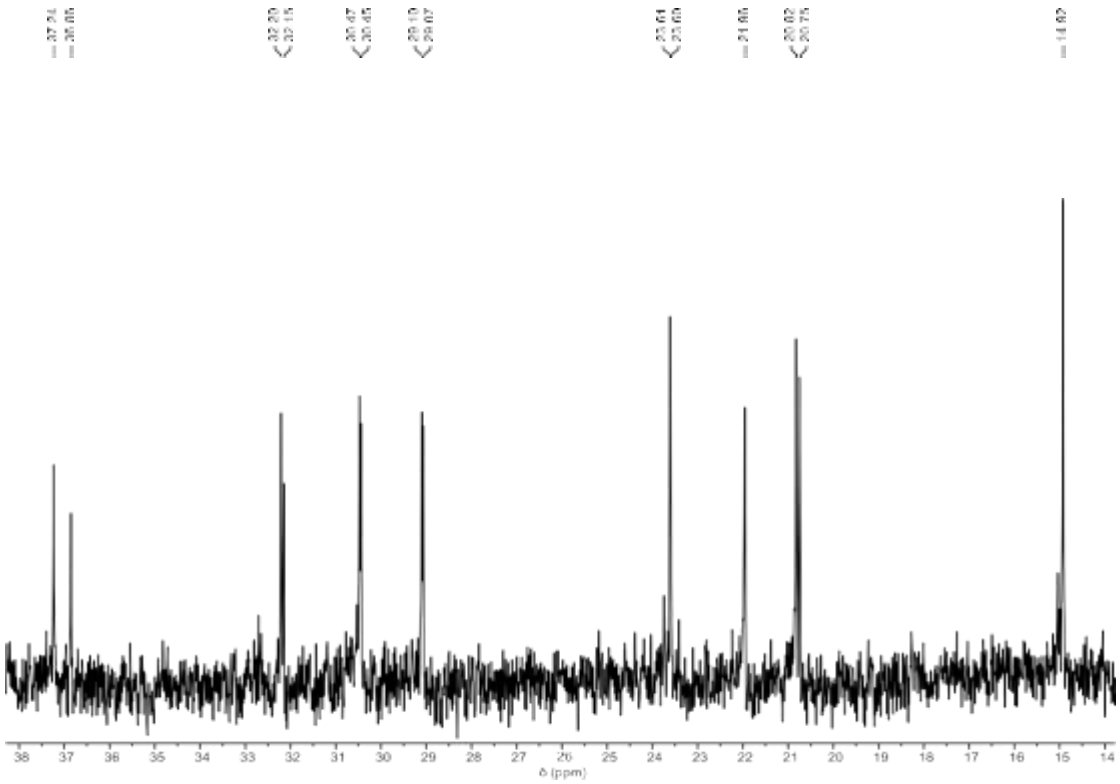


Figure S16 – ^{13}C NMR (CS_2 (D_2O log tube), 126 MHz) spectrum of **10** – Selected region.

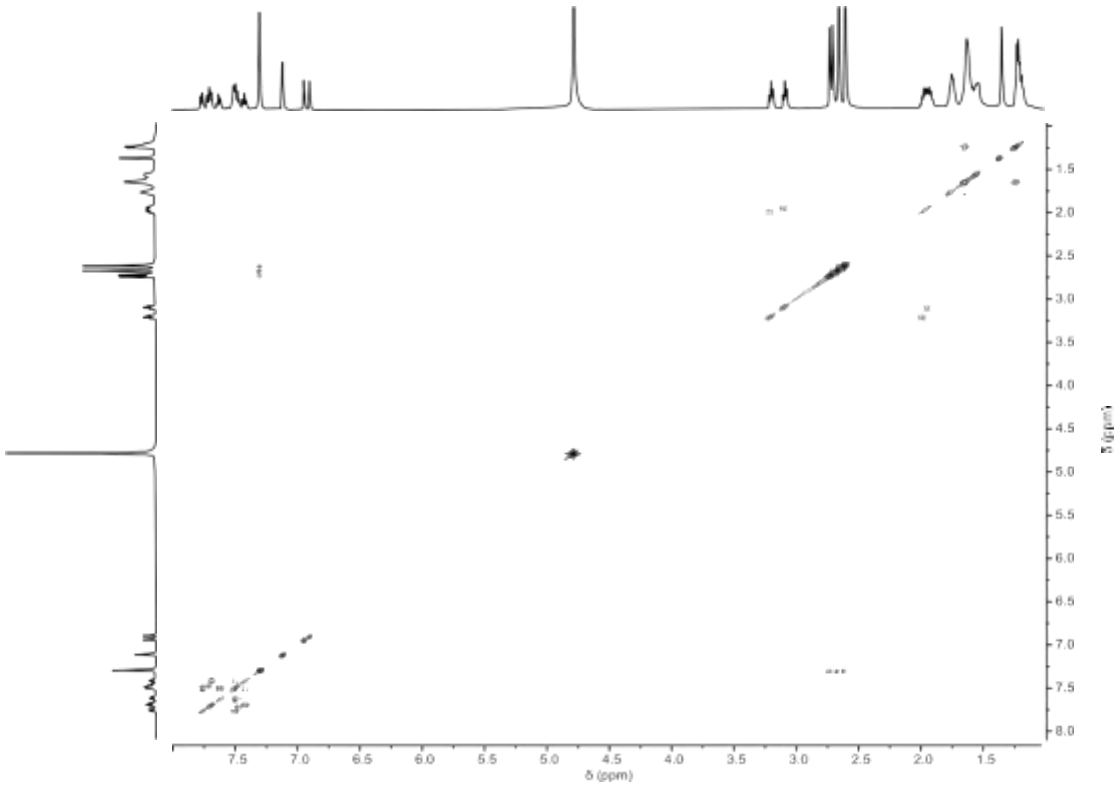


Figure S17 – $^{1}H/^{1}H$ COSY NMR (CS_2 (D_2O log tube), 500/500 MHz) spectrum of **10**.

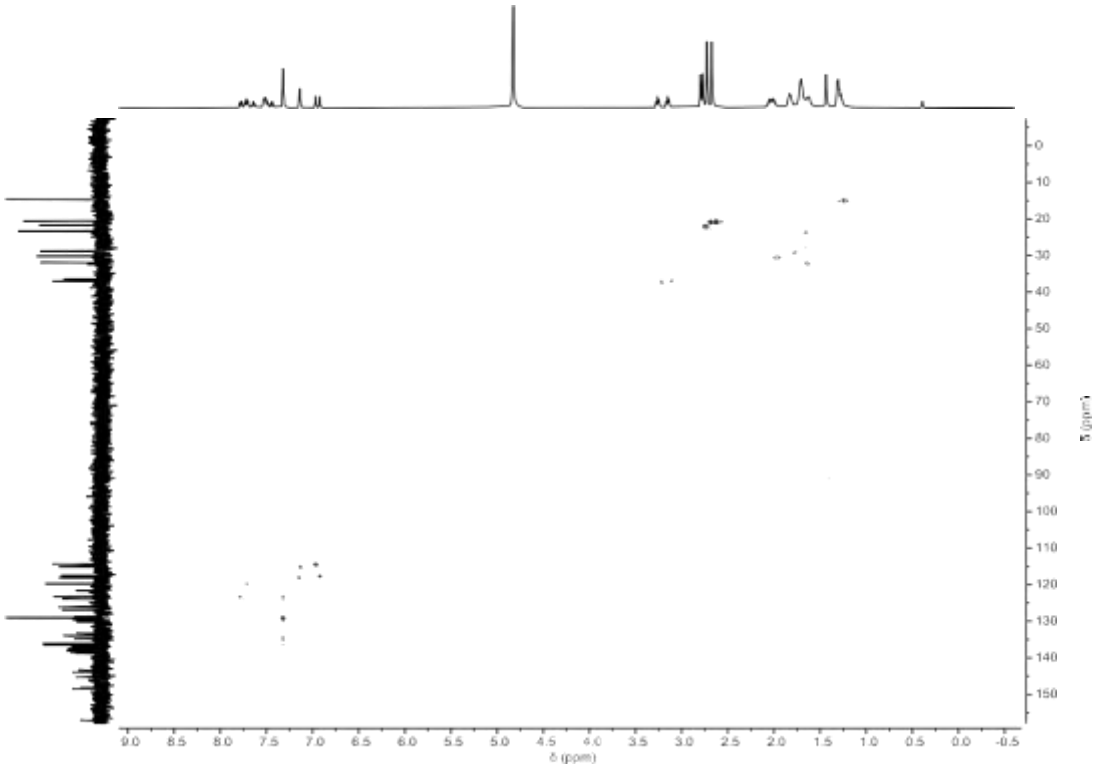


Figure S18 – $^{1}H/^{13}C$ HSQC NMR (CS_2 (D_2O log tube), 500/126 MHz) spectrum of **10**.

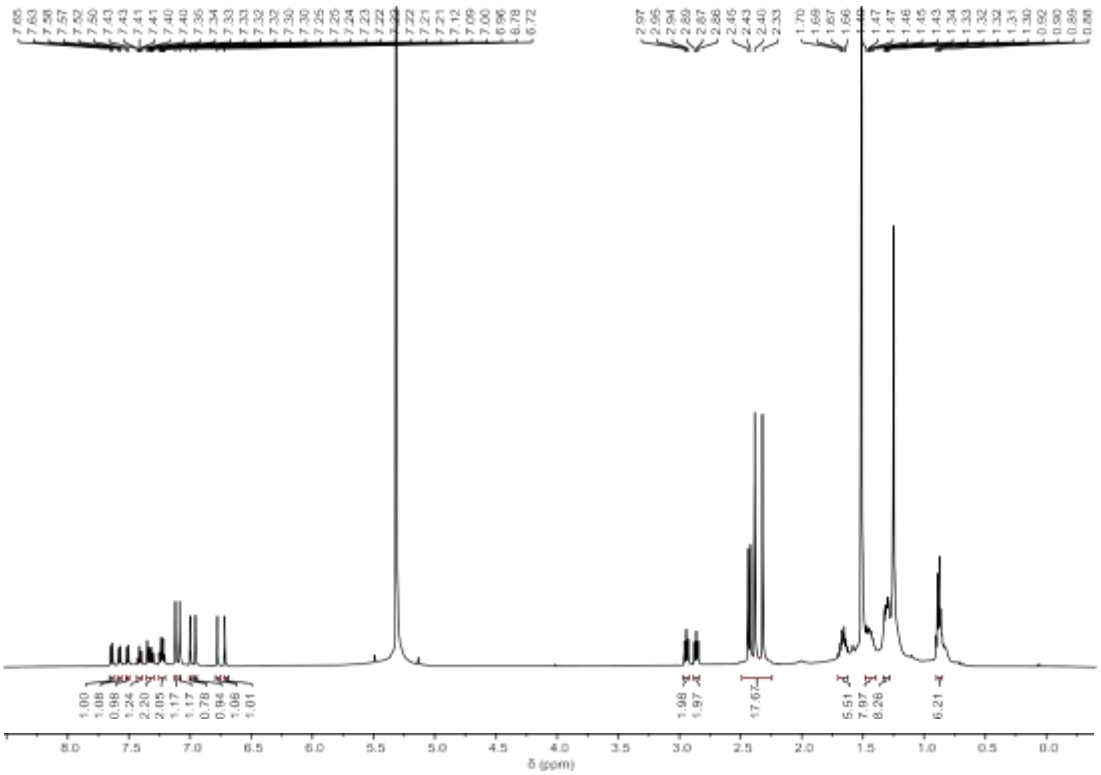


Figure S1G – ^{1}H NMR (CD_2Cl_2, 500 MHz) spectrum of **10**.

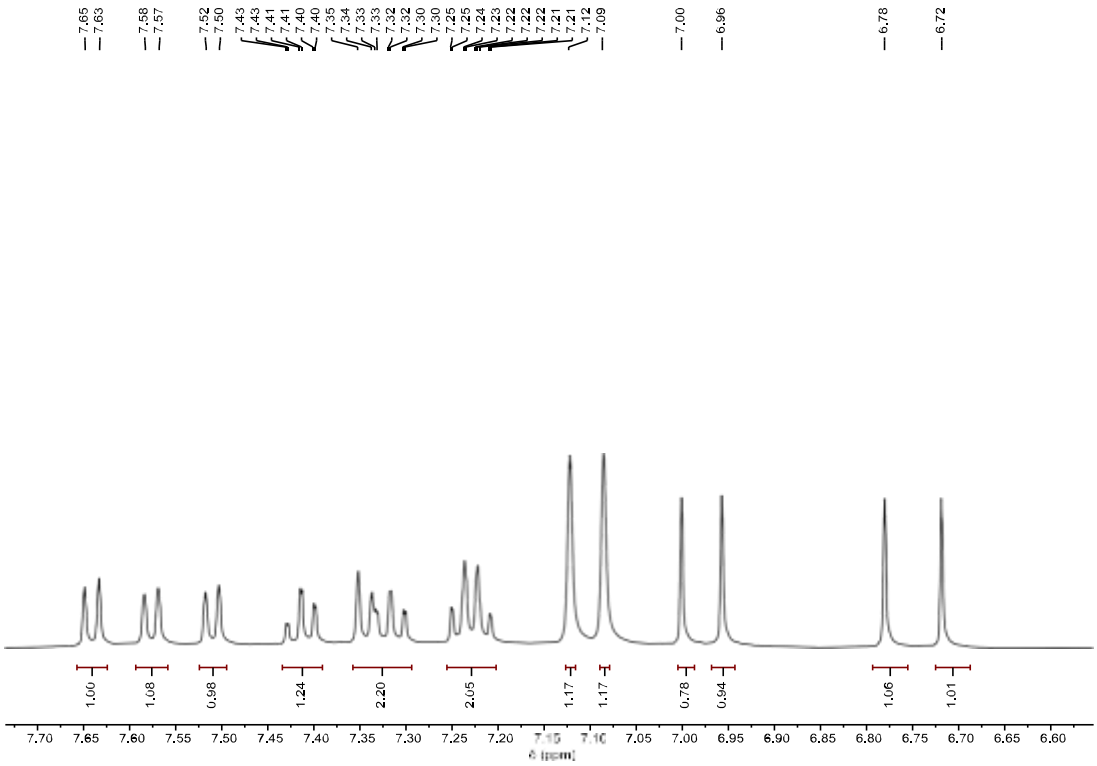


Figure S20 – ^{1}H NMR (CD_2Cl_2, 500 MHz) spectrum of **10** – Selected region.

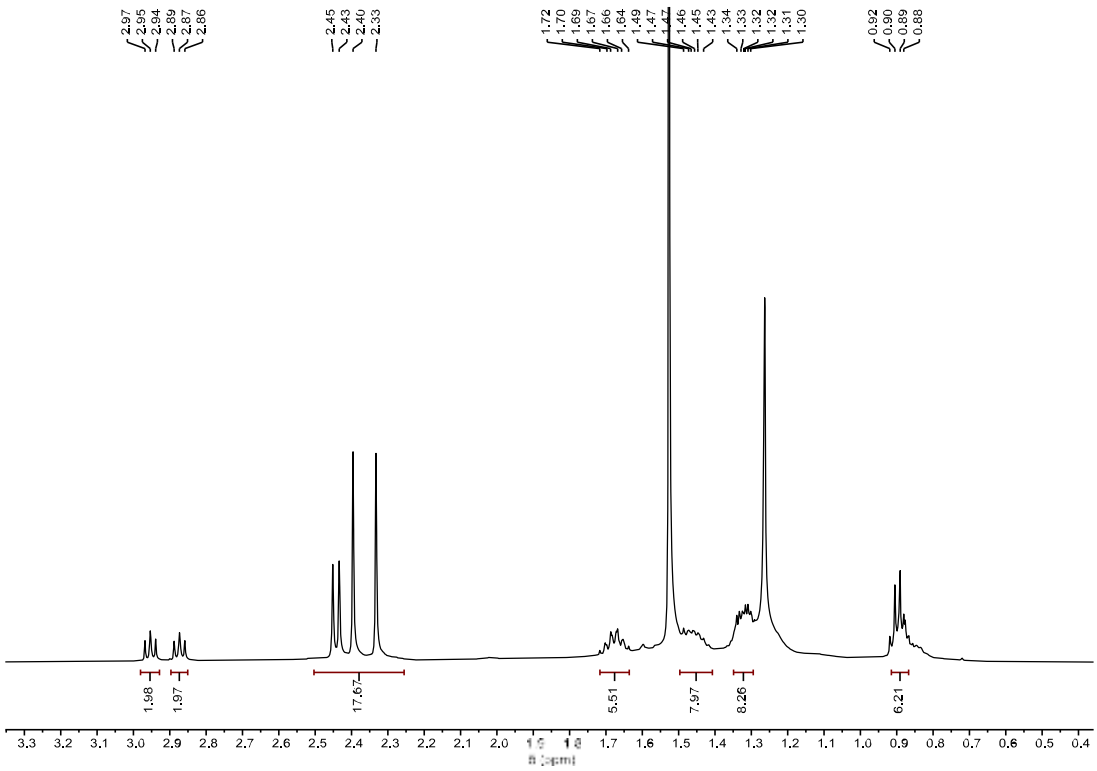


Figure S21 – ^{1}H NMR (CD_2Cl_2, 500 MHz) spectrum of **10** – Selected region.

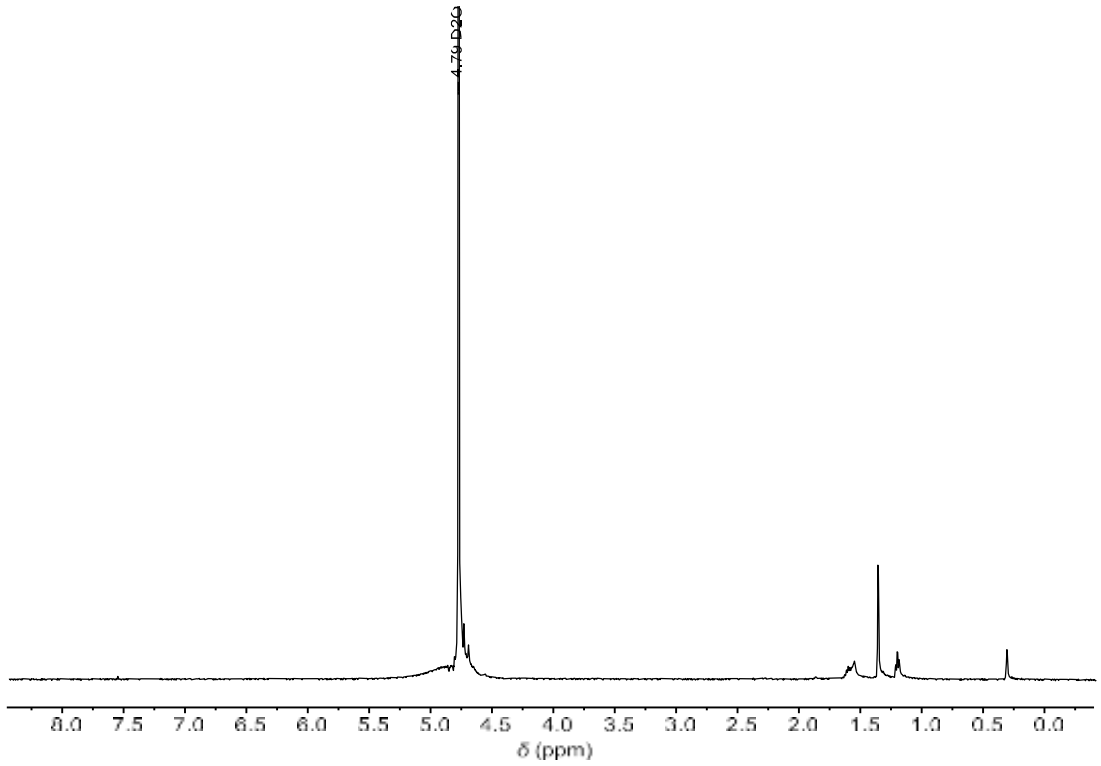


Figure S22 – ^{1}H NMR (CS_2 (D_2O log tube), 500 MHz) spectrum of blank CS_2.

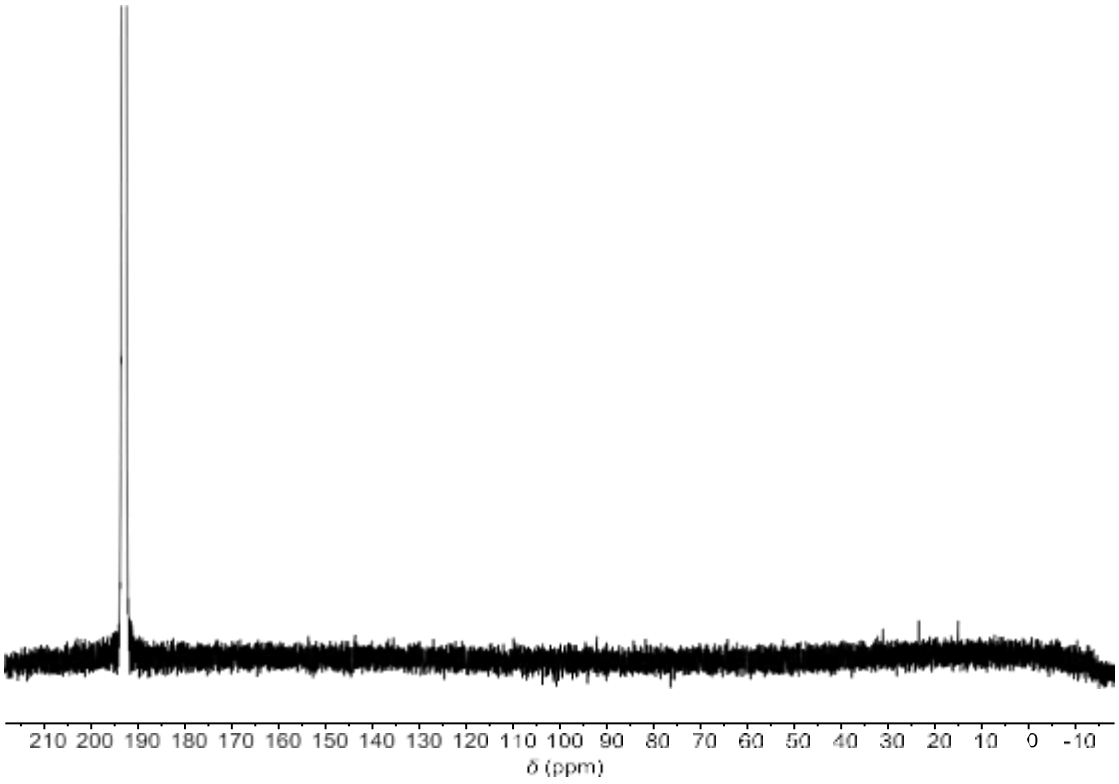


Figure S23 – ^{13}C NMR (CS_2 (D_2O log tube), 126 MHz) spectrum of blank CS_2.

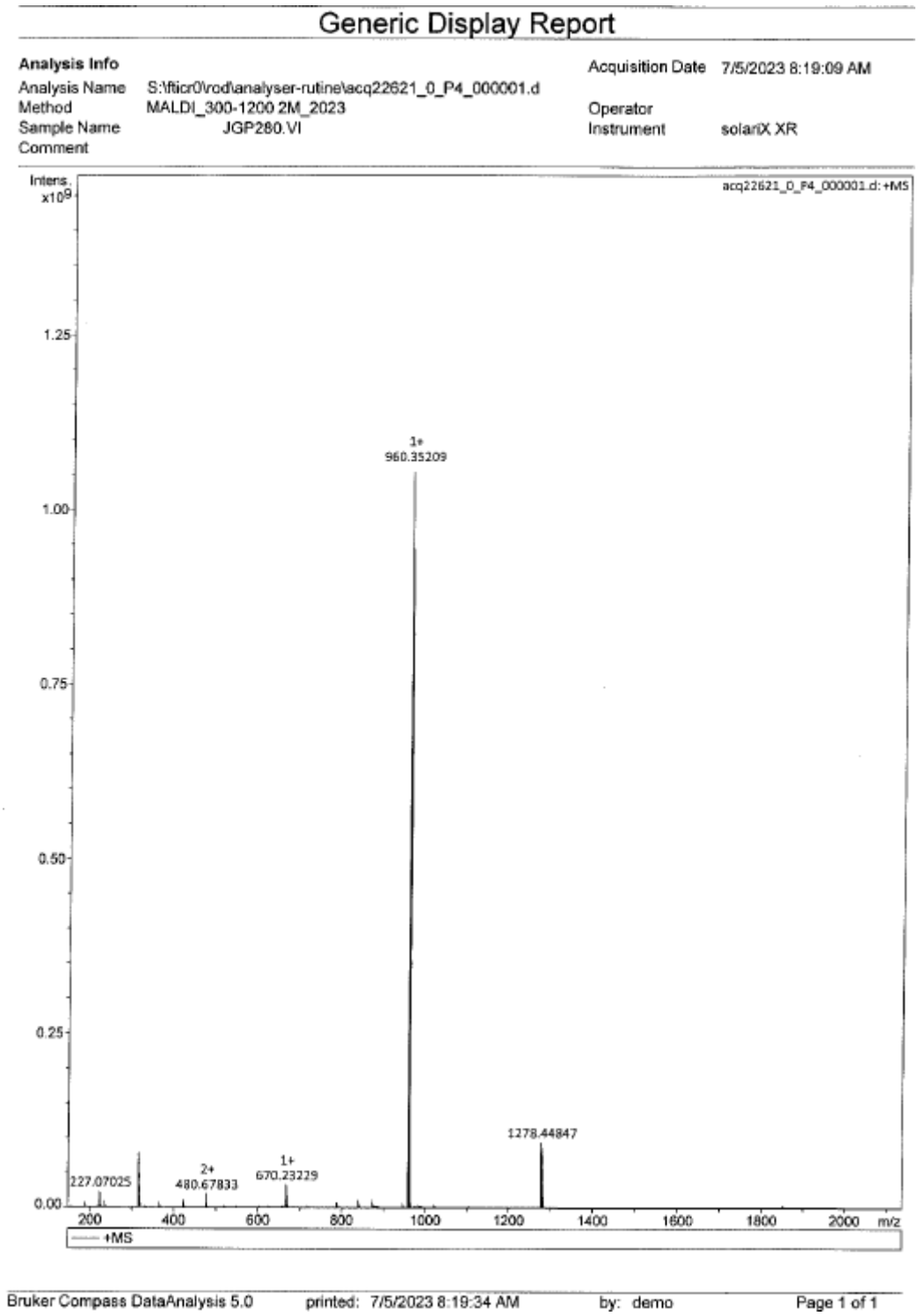


Figure S24 - HRMS (MALDI$^+$, dithranol) spectrum of **10**.

Electrochemistry

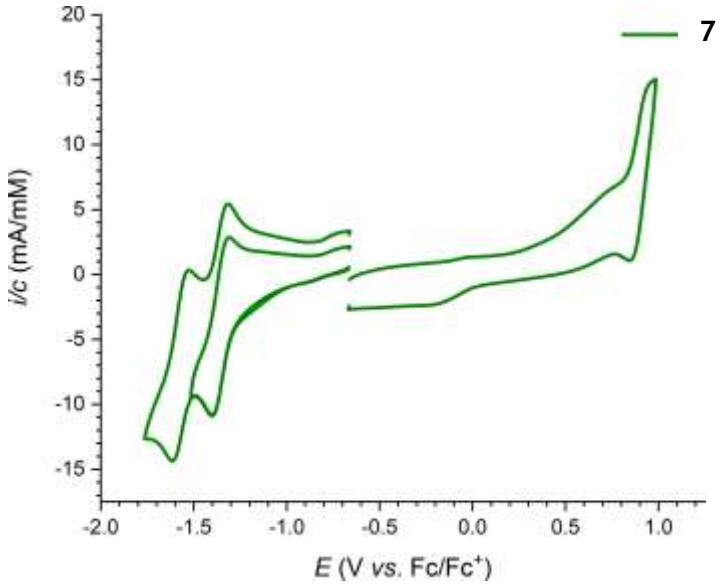


Figure S25 – Cyclic voltammograms of **7** (0.5 mM). Potentials *vs*. Fc/Fc^+ in CH_2Cl_2 with 0.1 M nBu_4NPF_6 as supporting electrolyte. Pt (1.6 mm) as working electrode, Pt wire as counter electrode, and Ag wire as reference electrode.

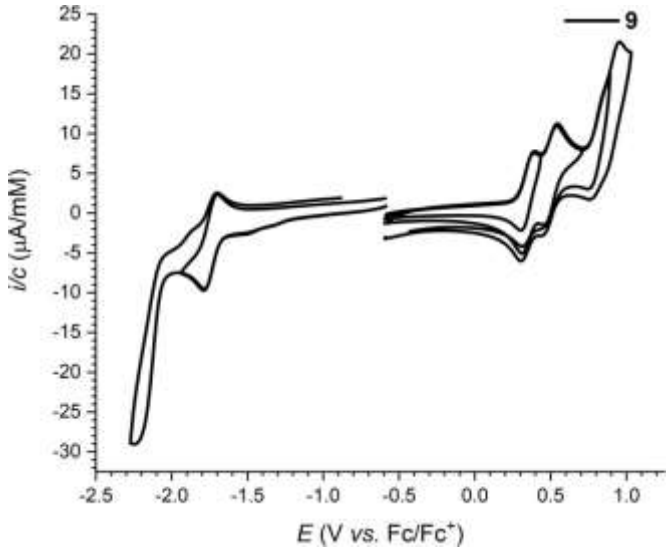


Figure S26 – Cyclic voltammograms of **G** (0.5 mM). Potentials *vs*. Fc/Fc^+ in CH_2Cl_2 with 0.1 M nBu_4NPF_6 as supporting electrolyte. Pt (1.6 mm) as working electrode, Pt wire as counter electrode, and Ag wire as reference electrode.

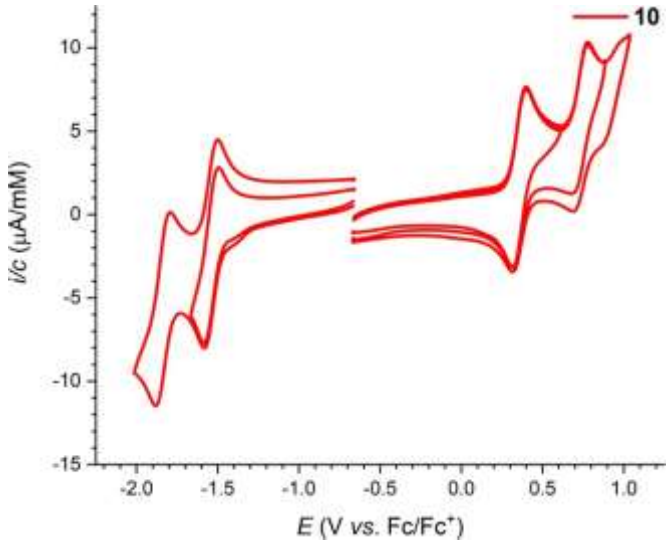


Figure S27 – Cyclic voltammograms of **10** (0.5 мм). Potentials vs. Fc/Fc^+ in CH_2Cl_2 with 0.1 м nBu_4NPF_6 as supporting electrolyte. Pt (1.6 mm) as working electrode, Pt wire as counter electrode, and Ag wire as reference electrode.

UV/Vis absorption spectroscopy

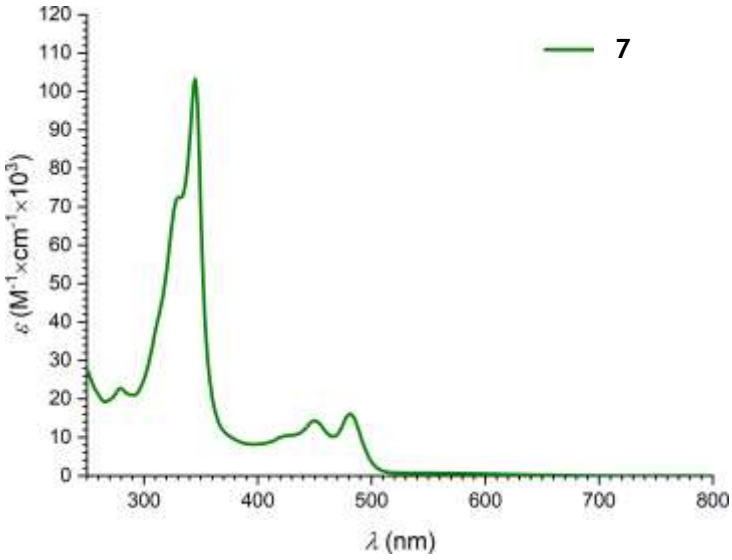


Figure S28 – UV/Vis absorption spectrum of **7** in CH_2Cl_2 at 25 °C.

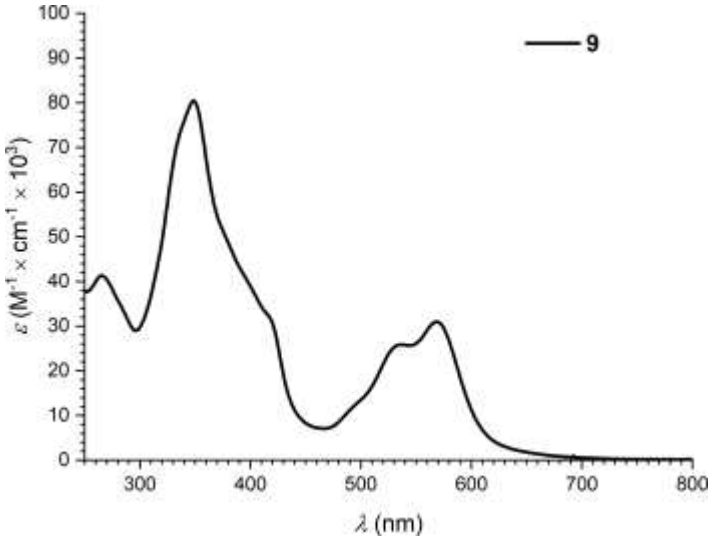


Figure S2G – UV/Vis absorption spectrum of **G** in CH_2Cl_2 at 25 °C.

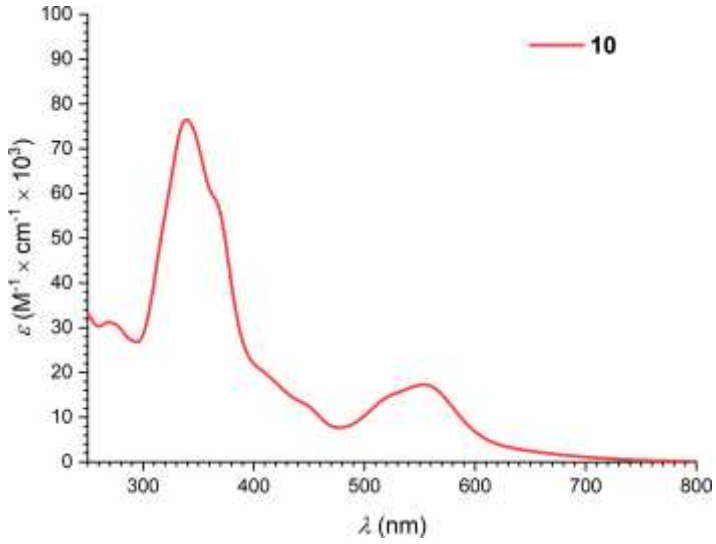


Figure S30 – UV/Vis absorption spectrum of **10** in CH_2Cl_2 at 25 °C.

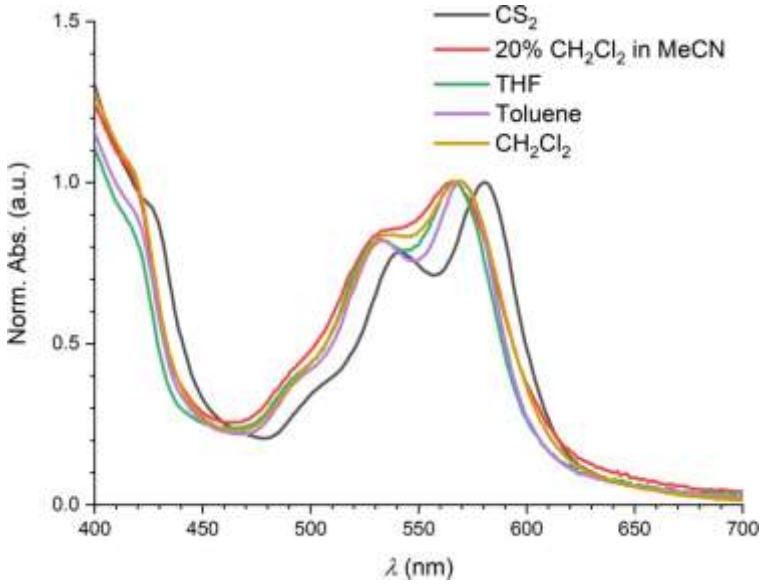


Figure S31 – UV/Vis absorption spectra of **G** in different solvents at 25 °C.

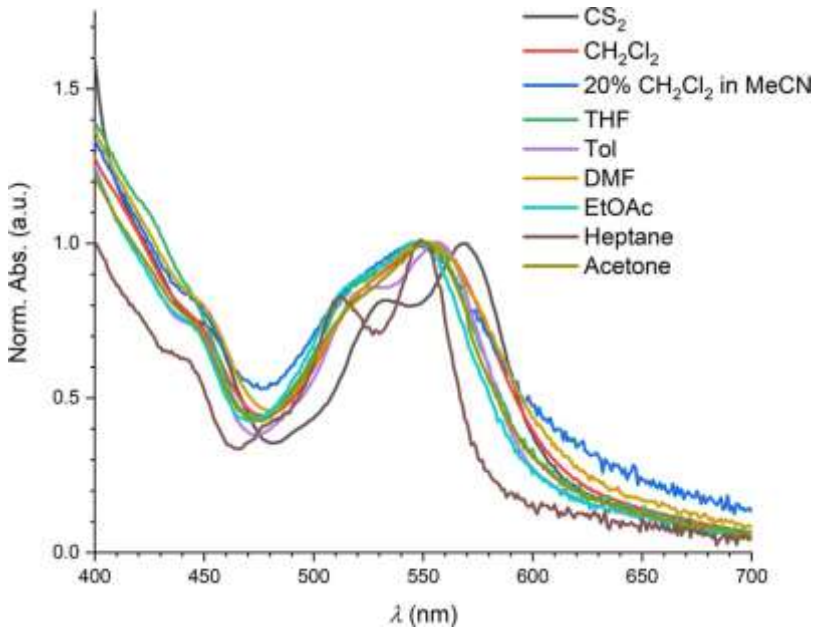


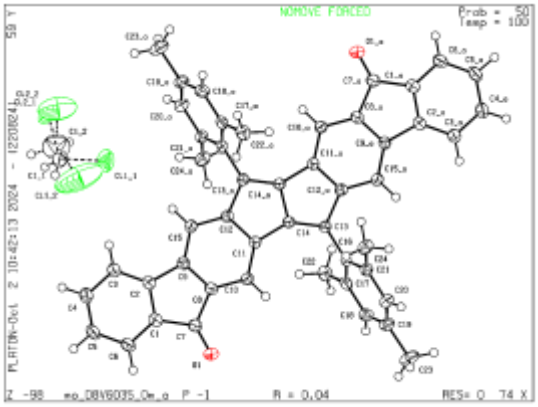
Figure S32 – UV/Vis absorption spectra of **10** in different solvents at 25 °C.

Tabel S1 – Longest-wavelength absorption maxima in different solvents at 25 °C.

Compound, Solvent	**λ_{max} (nm)**
G, CS_2	581
G, PhMe	570
G, THF	568
G, CH_2Cl_2	569
G, 20% CH_2Cl_2 in MeCN	566
10, CS_2	569
10, CH_2Cl_2	554
10, 20% CH_2Cl_2 in MeCN	551
10, THF	554
10, PhMe	557
10, DMF	554
10, EtOAc	548
10, *n*-Heptane	550
10, Acetone	551

Crystallographic Data

Compound **7**



Single crystals were obtained from diffusion of methanol into a solution of compound **7** in dichloromethane from a bilayer system. A yellow, block-shaped crystal was mounted on a MiTeGen micromount with perfluoroether oil. Data for compound **7** were collected from a shock-cooled single crystal at 100(2) K on a Bruker D8 VENTURE dual wavelength Mo/Cu three-circle diffractometer with a microfocus sealed X-ray tube using a mirror optics as monochromator and a Bruker PHOTON III detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.40B and a multi-scan absorption correction using SADABS 2016/2 was applied.[3,4] The structure was solved by direct methods with SHELXT and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/2.[5,6] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Disordered moieties were refined using bond lengths restraints and displacement parameter restraints. Some parts of the disorder model were introduced by the program DSR.[5,6] Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[7] CCDC 2388362 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[8]

Table S2. Crystal data and structure refinement for compound **7**

CCDC number	2388362
Empirical formula	$C_{49}H_{36}Cl_2O_2$
Formula weight	727.68
Temperature [K]	100(2)
Crystal system	triclinic
Space group (number)	□1 (2)
a [Å]	8.0184(9)
b [Å]	9.0834(7)
c [Å]	12.9502(12)
α [°]	87.358(4)
β [°]	77.624(6)
γ [°]	87.173(5)
Volume [Å^3]	919.57(15)
Z	1
ρ_{calc} [gcm^{-3}]	1.314
μ [mm^{-1}]	0.218
F(000)	380
Crystal size [mm^3]	0.078×0.135×0.142
Crystal colour	yellow
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.49 to 52.74 (0.80 Å)
Index ranges	−10 ≤ h ≤ 10 −11 ≤ k ≤ 11 −16 ≤ l ≤ 16
Reflections collected	39614
Independent reflections	3757 R_{int} = 0.0871 R_{sigma} = 0.0401
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	3757 / 59 / 285
Absorption correction T_{min}/T_{max} (method)	0.6602 / 0.7461 (multi-scan)
Goodness-of-fit on F^2	1.008
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0434 wR_2 = 0.1012
Final *R* indexes [all data]	R_1 = 0.0665 wR_2 = 0.1176
Largest peak/hole [eÅ^{-3}]	0.27/−0.28
Extinction coefficient	0.011(3)

Table S3. Atomic coordinates and U_{eq} [Å^2] for compound **7**.

Atom	*x*	*y*	*z*	U_{eq}
O1	0.05723(18)	0.61743(14)	0.85580(10)	0.0347(3)
C1	0.1333(2)	0.79223(19)	0.97329(14)	0.0261(4)
C2	0.2301(2)	0.91866(18)	0.95326(13)	0.0240(4)
C3	0.2541(2)	1.0000(2)	1.03610(14)	0.0284(4)
H3	0.319624	1.085775	1.023478	0.034
C4	0.1792(2)	0.9524(2)	1.13888(14)	0.0321(4)
H4	0.194010	1.006954	1.196893	0.039
C5	0.0837(2)	0.8273(2)	1.15791(14)	0.0329(4)
H5	0.033762	0.797688	1.228656	0.040
C6	0.0598(2)	0.7444(2)	1.07506(14)	0.0306(4)
H6	−0.004752	0.657992	1.087881	0.037
C7	0.1284(2)	0.72731(18)	0.87026(14)	0.0256(4)
C8	0.2311(2)	0.82539(17)	0.78764(13)	0.0222(4)
C9	0.2916(2)	0.93917(18)	0.83721(13)	0.0223(4)
C10	0.2699(2)	0.81218(17)	0.67853(13)	0.0216(3)
H10	0.226280	0.735440	0.645823	0.026
C11	0.3751(2)	0.91595(17)	0.61964(12)	0.0204(3)
C12	0.4329(2)	1.03429(17)	0.66931(13)	0.0212(3)
C13	0.4607(2)	0.87000(17)	0.41288(12)	0.0198(3)
C14	0.4501(2)	0.93393(16)	0.50688(13)	0.0206(3)
C15	0.3929(2)	1.04681(17)	0.77851(13)	0.0225(4)
H15	0.432881	1.125213	0.811568	0.027
C16	0.3894(2)	0.73054(17)	0.39107(12)	0.0198(3)
C17	0.2120(2)	0.71807(18)	0.40330(13)	0.0222(4)
C18	0.1498(2)	0.58484(19)	0.38272(14)	0.0263(4)
H18	0.029878	0.575811	0.392337	0.032
C19	0.2579(2)	0.46453(19)	0.34852(14)	0.0271(4)
C20	0.4321(2)	0.47978(18)	0.33665(14)	0.0262(4)
H20	0.507453	0.398485	0.312868	0.031
C21	0.5007(2)	0.60962(17)	0.35824(13)	0.0220(4)
C22	0.0916(2)	0.8483(2)	0.43600(14)	0.0290(4)
H22A	0.127773	0.933604	0.388768	0.043
H22B	0.093207	0.871851	0.508881	0.043
H22C	−0.024423	0.824326	0.431636	0.043
C23	0.1907(3)	0.3214(2)	0.32377(19)	0.0422(5)
H23A	0.189408	0.321390	0.248278	0.063
H23B	0.074425	0.310384	0.365541	0.063
H23C	0.264685	0.239110	0.341383	0.063
C24	0.6902(2)	0.61389(19)	0.35132(15)	0.0289(4)
H24A	0.750595	0.549194	0.295682	0.043
H24B	0.716430	0.580131	0.419259	0.043
H24C	0.726953	0.715111	0.334521	0.043
Cl1_1	0.4180(13)	1.4223(10)	0.9327(6)	0.0641(16)
Cl2_1	0.5857(15)	1.6055(9)	1.0493(7)	0.076(3)
C1_1	0.4373(10)	1.4702(8)	1.0590(5)	0.0472(19)
H1A_1	0.325021	1.506944	1.099380	0.057
H1B_1	0.473821	1.381935	1.097563	0.057
Cl1_2	0.4688(11)	1.3449(10)	1.0349(18)	0.179(9)
Cl2_2	0.6371(16)	1.5970(17)	1.0214(17)	0.118(7)
C1_2	0.4266(19)	1.5347(14)	1.052(3)	0.093(10)

H1A_2	0.368661	1.555727	1.125905	0.111
H1B_2	0.357308	1.578243	1.002959	0.111

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table S4 Anisotropic displacement parameters [Å^2] for compound **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0434(8)	0.0291(7)	0.0311(7)	0.0008(5)	−0.0043(6)	−0.0155(6)
C1	0.0252(9)	0.0277(9)	0.0244(9)	0.0020(7)	−0.0039(7)	−0.0021(7)
C2	0.0235(9)	0.0260(8)	0.0214(9)	0.0011(6)	−0.0031(7)	−0.0015(7)
C3	0.0300(9)	0.0321(9)	0.0230(9)	−0.0011(7)	−0.0041(7)	−0.0059(7)
C4	0.0343(10)	0.0399(10)	0.0226(9)	−0.0025(8)	−0.0058(8)	−0.0055(8)
C5	0.0346(10)	0.0426(11)	0.0204(9)	0.0050(7)	−0.0031(7)	−0.0077(8)
C6	0.0335(10)	0.0325(9)	0.0250(9)	0.0059(7)	−0.0048(8)	−0.0084(8)
C7	0.0258(9)	0.0238(8)	0.0258(9)	0.0012(7)	−0.0026(7)	−0.0025(7)
C8	0.0220(8)	0.0211(8)	0.0226(9)	0.0011(6)	−0.0029(7)	−0.0016(6)
C9	0.0215(8)	0.0233(8)	0.0210(8)	−0.0017(6)	−0.0021(6)	−0.0002(6)
C10	0.0218(8)	0.0194(8)	0.0234(8)	−0.0023(6)	−0.0041(7)	−0.0017(6)
C11	0.0218(8)	0.0196(8)	0.0192(8)	−0.0022(6)	−0.0029(6)	−0.0009(6)
C12	0.0187(8)	0.0197(8)	0.0245(9)	−0.0011(6)	−0.0029(6)	−0.0012(6)
C13	0.0194(8)	0.0180(7)	0.0213(8)	−0.0017(6)	−0.0023(6)	−0.0005(6)
C14	0.0202(8)	0.0178(8)	0.0226(8)	−0.0012(6)	−0.0017(6)	−0.0019(6)
C15	0.0234(8)	0.0221(8)	0.0220(8)	−0.0035(6)	−0.0038(7)	−0.0021(6)
C16	0.0216(8)	0.0206(8)	0.0171(8)	−0.0002(6)	−0.0031(6)	−0.0036(6)
C17	0.0203(8)	0.0274(8)	0.0183(8)	0.0005(6)	−0.0029(6)	−0.0019(6)
C18	0.0195(8)	0.0316(9)	0.0288(9)	0.0028(7)	−0.0066(7)	−0.0077(7)
C19	0.0283(9)	0.0252(9)	0.0309(9)	0.0011(7)	−0.0123(7)	−0.0078(7)
C20	0.0271(9)	0.0216(8)	0.0312(10)	−0.0035(7)	−0.0084(7)	−0.0014(7)
C21	0.0202(8)	0.0229(8)	0.0229(8)	−0.0027(6)	−0.0045(6)	−0.0012(6)
C22	0.0229(9)	0.0347(10)	0.0284(9)	−0.0024(7)	−0.0041(7)	0.0028(7)
C23	0.0439(12)	0.0317(10)	0.0570(14)	−0.0033(9)	−0.0206(10)	−0.0151(9)
C24	0.0209(9)	0.0278(9)	0.0386(10)	−0.0077(7)	−0.0064(7)	−0.0008(7)
Cl1_1	0.097(3)	0.060(4)	0.043(2)	−0.003(2)	−0.0318(18)	−0.003(3)
Cl2_1	0.132(5)	0.047(3)	0.061(4)	0.003(2)	−0.041(3)	−0.043(3)
C1_1	0.074(5)	0.035(4)	0.032(3)	−0.004(3)	−0.010(3)	−0.007(3)
Cl1_2	0.080(6)	0.085(6)	0.38(3)	−0.032(8)	−0.074(8)	0.001(4)
Cl2_2	0.056(5)	0.081(7)	0.217(19)	0.017(8)	−0.031(7)	−0.003(4)
C1_2	0.106(18)	0.071(18)	0.103(18)	0.010(11)	−0.029(11)	0.004(10)

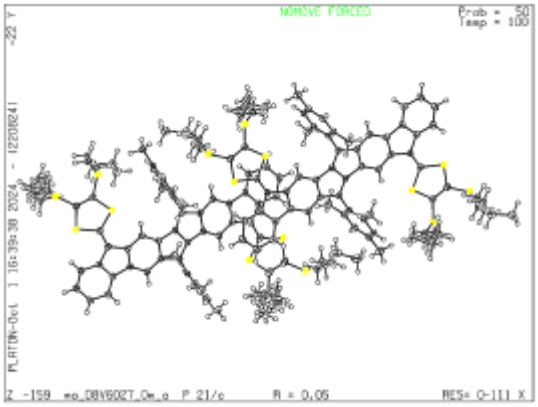
Table S5. Bond lengths and angles for compound **7**.

Atom-Atom	**Length [Å]**
O1–C7	1.215(2)
C1–C6	1.383(2)
C1–C2	1.401(2)
C1–C7	1.492(2)
C2–C3	1.382(2)
C2–C9	1.484(2)
C3–C4	1.396(3)
C4–C5	1.385(3)
C5–C6	1.390(3)
C7–C8	1.491(2)
C8–C10	1.390(2)
C8–C9	1.400(2)
C9–C15	1.392(2)
C10–C11	1.385(2)
C11–C12	1.423(2)
C11–C14	1.460(2)
C12–C15	1.390(2)
C12–C13$^{\#1}$	1.488(2)
C13–C14	1.357(2)
C13–C16	1.479(2)
C14–C14$^{\#1}$	1.458(3)
C16–C21	1.403(2)
C16–C17	1.406(2)
C17–C18	1.390(2)
C17–C22	1.507(2)
C18–C19	1.389(2)
C19–C20	1.385(2)

C19–C23	1.505(2)
C20–C21	1.390(2)
C21–C24	1.505(2)
Cl1_1–C1_1	1.752(7)
Cl2_1–C1_1	1.734(7)
Cl1_2–C1_2	1.755(9)
Cl2_2–C1_2	1.764(9)
Atom-Atom-Atom	**Angle [˚]**
C6–C1–C2	121.82(16)
C6–C1–C7	129.50(16)
C2–C1–C7	108.68(14)
C3–C2–C1	120.21(16)
C3–C2–C9	131.20(16)
C1–C2–C9	108.59(15)
C2–C3–C4	118.09(17)
C5–C4–C3	121.29(17)
C4–C5–C6	120.98(17)
C1–C6–C5	117.61(17)
O1–C7–C8	126.80(16)
O1–C7–C1	127.78(16)
C8–C7–C1	105.43(14)
C10–C8–C9	122.37(15)
C10–C8–C7	128.76(15)
C9–C8–C7	108.85(14)
C15–C9–C8	121.11(15)
C15–C9–C2	130.45(15)
C8–C9–C2	108.44(14)
C11–C10–C8	116.98(15)
C10–C11–C12	120.85(15)
C10–C11–C14	132.97(15)
C12–C11–C14	106.17(14)
C15–C12–C11	121.66(15)
C15–C12–C13$^{\#1}$	129.15(15)
C11–C12–C13$^{\#1}$	109.16(14)
C14–C13–C16	129.07(14)
C14–C13–C12$^{\#1}$	106.70(13)
C16–C13–C12$^{\#1}$	124.20(14)
C13–C14–C14$^{\#1}$	110.85(17)
C13–C14–C11	142.09(15)
C14$^{\#1}$–C14–C11	107.05(17)
C12–C15–C9	116.95(15)
C21–C16–C17	120.00(14)
C21–C16–C13	119.24(14)
C17–C16–C13	120.76(14)
C18–C17–C16	119.05(15)
C18–C17–C22	120.52(15)
C16–C17–C22	120.42(15)
C19–C18–C17	121.90(16)
C20–C19–C18	117.94(15)
C20–C19–C23	120.15(16)
C18–C19–C23	121.91(16)
C19–C20–C21	122.44(16)
C20–C21–C16	118.65(15)
C20–C21–C24	119.25(15)
C16–C21–C24	122.02(14)
Cl2_1–C1_1–Cl1_1	110.2(5)
Cl1_2–C1_2–Cl2_2	99.9(9)

Symmetry transformations used to generate equivalent atoms:
#1: 1-X, 2-Y, 1-Z;

Conpound G



Single crystals of compound **G** were grown by slow diffusion of heptane into a solution of the compound in carbon disulfide. A black, block-shaped crystal was mounted on a MiTeGen micromount with perfluoroether oil. Data for compound **G** were collected from a shock-cooled single crystal at 100(2) K on a Bruker D8 VENTURE dual wavelength Mo/Cu three-circle diffractometer with a microfocus sealed X-ray tube using a mirror optics as monochromator and a Bruker PHOTON III detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.40B and a multi-scan absorption correction using SADABS 2016/2 was applied.[1,2] The structure was solved by direct methods with SHELXT and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/2.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Disordered moieties were refined using bond lengths restraints and displacement parameter restraints. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[7] CCDC 2388363 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[8]

Table S6. Crystal data and structure refinement for compound **G**.

CCDC number	2388363
Empirical formula	$C_{78}H_{86}S_8$
Formula weight	1279.94
Temperature [K]	100(2)
Crystal system	monoclinic
Space group (number)	□2_1/□ (14)
a [Å]	22.963(2)
b [Å]	16.7610(13)
c [Å]	26.077(3)
α [°]	90
β [°]	96.82
γ [°]	90
Volume [Å^3]	9965.9(16)
Z	6
ρ_{calc} [gcm^{-3}]	1.280
μ [mm^{-1}]	0.313
F(000)	4092
Crystal size [mm^3]	0.070×0.152×0.161
Crystal colour	black
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	2.89 to 56.56 (0.75 Å)
Index ranges	−30 ≤ h ≤ 30 −22 ≤ k ≤ 22 −34 ≤ l ≤ 34
Reflections collected	379747
Independent reflections	24742 R_{int} = 0.2217 R_{sigma} = 0.0848
Completeness to θ = 25.242°	100.0 %
Data / Restraints / Parameters	24742 / 0 / 1216
Absorption correction T_{min}/T_{max} (method)	0.6951 / 0.7457 (multi-scan)
Goodness-of-fit on F^2	1.008
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0550 wR_2 = 0.1291
Final *R* indexes [all data]	R_1 = 0.1009 wR_2 = 0.1586
Largest peak/hole [eÅ^{-3}]	0.49/−0.42
Extinction coefficient	0.00069(12)

Table S7. Atomic coordinates and U_{eq} [Å^2] for compound **G**.

Atom	*x*	*y*	*z*	U_{eq}
S1_1	0.55095(3)	0.73137(4)	0.50146(3)	0.02390(15)
C1_1	0.42123(11)	0.52178(14)	0.46124(10)	0.0197(5)
S2_1	0.48607(3)	0.73895(4)	0.59063(3)	0.02207(14)
C2_1	0.41529(12)	0.46989(15)	0.41954(11)	0.0236(6)
H2_1	0.386400	0.429066	0.417201	0.028
S3_1	0.16154(3)	0.24965(4)	0.72339(3)	0.02610(15)
C3_1	0.45189(12)	0.47815(16)	0.38135(11)	0.0252(6)
H3_1	0.448838	0.442035	0.353079	0.030
S4_1	0.11381(3)	0.24340(4)	0.82169(3)	0.02779(16)
C4_1	0.49316(12)	0.53931(15)	0.38430(11)	0.0230(5)
H4_1	0.517936	0.544511	0.357790	0.028
S5_1	0.62899(3)	0.87080(4)	0.53605(3)	0.02953(16)
C5_1	0.49885(11)	0.59280(15)	0.42517(10)	0.0224(5)
H5_1	0.526932	0.634586	0.426440	0.027
S6_1	0.55232(3)	0.87533(4)	0.64088(3)	0.02550(15)
C6_1	0.46296(11)	0.58463(14)	0.46431(10)	0.0190(5)
S7_1	0.07573(3)	0.13011(4)	0.67166(3)	0.03231(17)
C7_1	0.45920(11)	0.62879(15)	0.51268(10)	0.0201(5)
S8_1	0.02522(3)	0.11636(4)	0.78642(4)	0.03537(19)
C8_1	0.41378(11)	0.58878(14)	0.53854(10)	0.0189(5)
C9_1	0.39159(11)	0.52331(14)	0.50768(10)	0.0192(5)
C10_1	0.39496(11)	0.60148(14)	0.58712(10)	0.0201(5)
H10_1	0.408469	0.645945	0.607789	0.024
C11_1	0.35617(11)	0.54723(14)	0.60391(10)	0.0192(5)
C12_1	0.33507(11)	0.47978(14)	0.57360(10)	0.0201(5)
C13_1	0.35217(11)	0.46854(15)	0.52513(11)	0.0213(5)
H13_1	0.337638	0.424880	0.504158	0.026
C14_1	0.33374(11)	0.53884(14)	0.65364(10)	0.0200(5)
C15_1	0.29875(11)	0.46635(14)	0.65124(11)	0.0209(5)
C16_1	0.29928(11)	0.42982(15)	0.60499(10)	0.0205(5)
C17_1	0.33965(11)	0.56939(14)	0.70203(10)	0.0182(5)
C18_1	0.30560(11)	0.51743(14)	0.73379(10)	0.0196(5)
C19_1	0.28061(11)	0.45348(15)	0.70233(10)	0.0208(5)
C20_1	0.29545(11)	0.52299(14)	0.78496(10)	0.0192(5)
H20_1	0.312281	0.564815	0.806417	0.023
C21_1	0.25983(11)	0.46546(15)	0.80414(10)	0.0206(5)
C22_1	0.23501(11)	0.40180(15)	0.77258(11)	0.0210(5)
C23_1	0.24655(11)	0.39537(15)	0.72131(11)	0.0216(5)
H23_1	0.231363	0.352214	0.700193	0.026
C24_1	0.23888(11)	0.45918(15)	0.85434(11)	0.0211(5)
C25_1	0.20034(11)	0.39305(15)	0.85369(11)	0.0213(5)
C26_1	0.19679(11)	0.35490(15)	0.80271(11)	0.0208(5)
C27_1	0.17251(12)	0.37776(17)	0.89746(11)	0.0252(6)
H27_1	0.146448	0.333822	0.897917	0.030
C28_1	0.18314(12)	0.42713(17)	0.94033(11)	0.0275(6)
H28_1	0.163529	0.417055	0.969761	0.033
C29_1	0.22196(12)	0.49112(17)	0.94106(11)	0.0279(6)
H29_1	0.229160	0.523598	0.971000	0.033
C30_1	0.25018(12)	0.50736(16)	0.89780(11)	0.0245(6)
H30_1	0.276803	0.550776	0.897985	0.029

C31_1	0.49352(11)	0.69121(14)	0.53198(10)	0.0208(5)
C32_1	0.57214(12)	0.80578(15)	0.54721(11)	0.0235(6)
C33_1	0.54195(11)	0.80893(15)	0.58820(11)	0.0223(5)
C34_1	0.27451(12)	0.34893(15)	0.59347(10)	0.0209(5)
C35_1	0.21829(12)	0.33902(15)	0.56774(11)	0.0238(6)
C36_1	0.19457(13)	0.26196(16)	0.56335(11)	0.0262(6)
H36_1	0.156476	0.254710	0.545361	0.031
C37_1	0.22484(13)	0.19624(16)	0.58434(11)	0.0275(6)
C38_1	0.28142(13)	0.20746(16)	0.60901(11)	0.0261(6)
H38_1	0.303016	0.162547	0.622987	0.031
C39_1	0.30720(12)	0.28263(15)	0.61373(10)	0.0225(5)
C40_1	0.37685(11)	0.63845(14)	0.72082(10)	0.0190(5)
C41_1	0.35702(12)	0.71650(15)	0.71034(11)	0.0219(5)
C42_1	0.39430(12)	0.77947(15)	0.72634(11)	0.0232(6)
H42_1	0.381355	0.832578	0.719193	0.028
C43_1	0.45006(12)	0.76700(15)	0.75254(11)	0.0225(5)
C44_1	0.46839(11)	0.68894(15)	0.76240(11)	0.0221(5)
H44_1	0.506264	0.679539	0.780300	0.027
C45_1	0.43267(11)	0.62400(14)	0.74672(10)	0.0199(5)
C46_1	0.16232(11)	0.29184(15)	0.78519(11)	0.0239(6)
C47_1	0.10120(12)	0.18611(15)	0.72634(12)	0.0268(6)
C48_1	0.08026(12)	0.18187(16)	0.77209(12)	0.0293(6)
C49_1	0.68626(13)	0.79942(18)	0.52602(12)	0.0319(7)
H49A_1	0.673131	0.766699	0.495206	0.038
H49B_1	0.721852	0.828871	0.519031	0.038
C50_1	0.70180(12)	0.74461(17)	0.57191(12)	0.0293(6)
H50A_1	0.666510	0.713758	0.578010	0.035
H50B_1	0.713309	0.777548	0.602977	0.035
C51_1	0.75134(12)	0.68660(17)	0.56495(12)	0.0304(6)
H51A_1	0.741091	0.655737	0.532773	0.037
H51B_1	0.787536	0.717127	0.561336	0.037
C52_1	0.76293(13)	0.62938(17)	0.61001(12)	0.0315(7)
H52A_1	0.727264	0.596912	0.612062	0.038
H52B_1	0.770134	0.660770	0.642304	0.038
C53_1	0.81466(14)	0.57340(17)	0.60693(13)	0.0346(7)
H53A_1	0.850109	0.605291	0.602868	0.042
H53B_1	0.806501	0.538862	0.576121	0.042
C54_1	0.82646(15)	0.5212(2)	0.65499(15)	0.0447(9)
H54A_1	0.791848	0.488414	0.658593	0.067
H54B_1	0.834954	0.555186	0.685543	0.067
H54C_1	0.860158	0.486499	0.651689	0.067
C55_1	0.61870(12)	0.83462(15)	0.67680(11)	0.0263(6)
H55A_1	0.651765	0.842590	0.656183	0.032
H55B_1	0.627533	0.865260	0.709246	0.032
C56_1	0.61531(12)	0.74667(15)	0.69013(11)	0.0236(6)
H56A_1	0.607101	0.715423	0.657863	0.028
H56B_1	0.582435	0.738121	0.710874	0.028
C57_1	0.67201(12)	0.71650(16)	0.72038(12)	0.0269(6)
H57A_1	0.676400	0.741142	0.755124	0.032
H57B_1	0.705555	0.734088	0.702600	0.032
C58_1	0.67447(12)	0.62580(16)	0.72638(12)	0.0282(6)
H58A_1	0.669568	0.601265	0.691600	0.034

H58B_1	0.713767	0.610713	0.743386	0.034
C59_1	0.62832(13)	0.59155(15)	0.75745(12)	0.0280(6)
H59A_1	0.588927	0.607164	0.740920	0.034
H59B_1	0.633692	0.614777	0.792598	0.034
C60_1	0.63140(13)	0.50100(16)	0.76159(13)	0.0340(7)
H60A_1	0.623311	0.477501	0.727068	0.051
H60B_1	0.602199	0.482145	0.783312	0.051
H60C_1	0.670656	0.485077	0.777058	0.051
C61_1	0.18236(13)	0.40932(17)	0.54690(13)	0.0343(7)
H61A_1	0.207592	0.447413	0.531479	0.051
H61B_1	0.164871	0.435279	0.575077	0.051
H61C_1	0.151190	0.391124	0.520565	0.051
C62_1	0.19748(15)	0.11411(16)	0.58177(13)	0.0349(7)
H62A_1	0.157466	0.117264	0.564007	0.052
H62B_1	0.196373	0.093688	0.616851	0.052
H62C_1	0.220850	0.078124	0.562771	0.052
C63_1	0.36762(12)	0.29308(17)	0.64144(12)	0.0305(6)
H63A_1	0.384701	0.240651	0.650527	0.046
H63B_1	0.365568	0.324283	0.672956	0.046
H63C_1	0.392144	0.321168	0.618969	0.046
C64_1	0.29679(12)	0.73194(16)	0.68303(12)	0.0297(6)
H64A_1	0.290459	0.789593	0.679424	0.045
H64B_1	0.267399	0.709057	0.703093	0.045
H64C_1	0.293197	0.707259	0.648728	0.045
C65_1	0.48906(12)	0.83640(16)	0.76949(12)	0.0289(6)
H65A_1	0.510561	0.853013	0.740995	0.043
H65B_1	0.516974	0.820554	0.799105	0.043
H65C_1	0.465095	0.880912	0.779419	0.043
C66_1	0.45497(12)	0.54020(15)	0.75637(12)	0.0267(6)
H66A_1	0.456184	0.512884	0.723284	0.040
H66B_1	0.428740	0.511299	0.776889	0.040
H66C_1	0.494507	0.541876	0.775207	0.040
C67_1	0.05793(13)	0.20903(17)	0.62451(12)	0.0314(6)
H67A_1	0.094176	0.239095	0.620328	0.038
H67B_1	0.043956	0.184392	0.590785	0.038
C68_1	0.01167(13)	0.26733(17)	0.63856(12)	0.0311(6)
H68A_1	0.022511	0.286715	0.674282	0.037
H68B_1	−0.026573	0.239661	0.637235	0.037
C73_1	−0.02528(13)	0.18560(18)	0.81164(13)	0.0339(7)
H73A_1	−0.058475	0.155040	0.822769	0.041
H73B_1	−0.004836	0.212380	0.842507	0.041
C74_1	−0.04945(13)	0.24899(17)	0.77299(12)	0.0302(6)
H74A_1	−0.016522	0.280445	0.762172	0.036
H74B_1	−0.069836	0.222613	0.741946	0.036
C75_1	−0.09177(13)	0.30464(18)	0.79554(12)	0.0334(7)
H75A_1	−0.074357	0.321602	0.830387	0.040
H75B_1	−0.128409	0.275285	0.799384	0.040
C76_1	−0.10661(14)	0.37853(18)	0.76241(13)	0.0370(7)
H76A_1	−0.131468	0.362416	0.730465	0.044
H76B_1	−0.069852	0.401185	0.752244	0.044
C77_1	−0.13846(16)	0.4431(2)	0.78951(15)	0.0470(9)
H77A_1	−0.113917	0.458335	0.821818	0.056

H77B_1	−0.142958	0.490836	0.767058	0.056
C78_1	−0.19826(16)	0.4182(2)	0.80247(16)	0.0556(11)
H78A_1	−0.223264	0.404194	0.770651	0.083
H78B_1	−0.216081	0.462420	0.819631	0.083
H78C_1	−0.194208	0.371871	0.825544	0.083
C69A_1	0.0057(6)	0.3409(9)	0.6001(6)	0.028(2)
H69A_1	0.045041	0.363724	0.597475	0.033
H69B_1	−0.010784	0.322597	0.565294	0.033
C70A_1	−0.0346(3)	0.4063(5)	0.6190(3)	0.0319(15)
H70A_1	−0.075182	0.385568	0.616731	0.038
H70B_1	−0.021460	0.418205	0.655783	0.038
C71A_1	−0.0343(3)	0.4835(4)	0.5877(3)	0.0354(17)
H71A_1	−0.053583	0.526055	0.605860	0.042
H71B_1	0.006792	0.499867	0.585924	0.042
C72A_1	−0.0651(3)	0.4760(4)	0.5334(3)	0.048(2)
H72A_1	−0.062975	0.527039	0.515342	0.072
H72B_1	−0.106303	0.461766	0.534704	0.072
H72C_1	−0.046052	0.434441	0.514880	0.072
C69B_1	−0.0059(9)	0.3229(12)	0.5970(10)	0.026(3)
H69C_1	−0.020415	0.291841	0.565813	0.032
H69D_1	0.029336	0.352475	0.589251	0.032
C70B_1	−0.0520(5)	0.3823(6)	0.6068(5)	0.033(2)
H70C_1	−0.038474	0.411891	0.638865	0.040
H70D_1	−0.088097	0.353082	0.612679	0.040
C71B_1	−0.0673(4)	0.4422(5)	0.5635(4)	0.039(3)
H71C_1	−0.106899	0.463854	0.566134	0.047
H71D_1	−0.068567	0.414134	0.529960	0.047
C72B_1	−0.0237(5)	0.5119(6)	0.5642(5)	0.052(3)
H72D_1	−0.037693	0.550392	0.537299	0.079
H72E_1	0.014842	0.491552	0.557818	0.079
H72F_1	−0.020308	0.538080	0.598043	0.079
S1_2	0.20618(3)	0.71519(4)	0.80949(3)	0.02387(15)
C1_2	0.11909(11)	0.56420(15)	0.79214(10)	0.0214(5)
S2_2	0.16548(3)	0.72728(4)	0.91085(3)	0.02716(16)
C2_2	0.08087(11)	0.49938(15)	0.79727(10)	0.0212(5)
S3_2	0.28945(3)	0.85049(4)	0.82383(3)	0.02542(15)
C3_2	0.06739(12)	0.44553(16)	0.75713(11)	0.0254(6)
H3_2	0.041400	0.402372	0.760847	0.030
S4_2	0.24019(3)	0.87214(4)	0.94167(3)	0.02577(15)
C4_2	0.09220(13)	0.45530(16)	0.71156(11)	0.0280(6)
H4_2	0.083065	0.418971	0.683804	0.034
C5_2	0.13048(13)	0.51836(16)	0.70656(12)	0.0280(6)
H5_2	0.147502	0.524339	0.675311	0.034
C6_2	0.14435(12)	0.57281(16)	0.74632(11)	0.0259(6)
H6_2	0.170726	0.615428	0.742371	0.031
C7_2	0.12439(11)	0.61069(15)	0.84035(10)	0.0204(5)
C8_2	0.08662(11)	0.57063(15)	0.87411(10)	0.0200(5)
C9_2	0.06155(11)	0.50270(15)	0.84822(10)	0.0214(5)
C10_2	0.15970(11)	0.67521(15)	0.85180(11)	0.0218(5)
C11_2	0.23651(11)	0.79153(15)	0.84967(11)	0.0235(6)
C12_2	0.21781(11)	0.79798(15)	0.89636(11)	0.0234(6)
C13_2	0.07412(11)	0.58800(15)	0.92458(10)	0.0220(5)

H13_2	0.089861	0.634165	0.942269	0.026
C14_2	0.03842(11)	0.53614(15)	0.94757(11)	0.0214(5)
C15_2	0.01468(11)	0.46604(15)	0.92182(11)	0.0215(5)
C16_2	0.02012(11)	0.57798(15)	1.04304(11)	0.0210(5)
C17_2	0.01779(11)	0.53589(15)	0.99836(11)	0.0227(5)
C18_2	0.02570(11)	0.44952(15)	0.87186(11)	0.0215(5)
H18_2	0.009519	0.403645	0.854123	0.026
C19_2	0.35599(12)	0.81694(15)	0.86249(11)	0.0250(6)
H19A_2	0.390061	0.843264	0.849698	0.030
H19B_2	0.354790	0.834227	0.898653	0.030
C20_2	0.36518(11)	0.72674(15)	0.86177(11)	0.0224(5)
H20A_2	0.331767	0.699967	0.875343	0.027
H20B_2	0.366135	0.708861	0.825692	0.027
C21_2	0.42184(12)	0.70241(15)	0.89397(11)	0.0247(6)
H21A_2	0.422088	0.723877	0.929358	0.030
H21B_2	0.455387	0.726175	0.878833	0.030
C22_2	0.42955(12)	0.61196(16)	0.89682(12)	0.0275(6)
H22A_2	0.427594	0.590459	0.861296	0.033
H22B_2	0.396648	0.588589	0.913075	0.033
C23_2	0.48744(13)	0.58591(17)	0.92740(12)	0.0300(6)
H23A_2	0.490760	0.610549	0.962126	0.036
H23B_2	0.487029	0.527283	0.931935	0.036
C24_2	0.54096(13)	0.60907(18)	0.90114(13)	0.0349(7)
H24A_2	0.540074	0.580449	0.868286	0.052
H24B_2	0.576756	0.594951	0.923603	0.052
H24C_2	0.540426	0.666678	0.894673	0.052
C25_2	0.26202(12)	0.81132(16)	0.99856(11)	0.0260(6)
H25A_2	0.276279	0.846993	1.027620	0.031
H25B_2	0.227029	0.782992	1.008079	0.031
C26_2	0.30933(12)	0.75034(16)	0.99178(11)	0.0248(6)
H26A_2	0.345664	0.778436	0.985298	0.030
H26B_2	0.296590	0.716791	0.961252	0.030
C27_2	0.32231(13)	0.69706(16)	1.03911(11)	0.0279(6)
H27A_2	0.285396	0.671840	1.046932	0.033
H27B_2	0.337455	0.730320	1.069130	0.033
C28_2	0.36702(12)	0.63195(17)	1.03146(12)	0.0298(6)
H28A_2	0.350812	0.596987	1.002650	0.036
H28B_2	0.403016	0.657183	1.021521	0.036
C29_2	0.38323(13)	0.58103(18)	1.07933(13)	0.0358(7)
H29A_2	0.394912	0.616452	1.109164	0.043
H29B_2	0.417467	0.547435	1.074026	0.043
C30_2	0.33330(14)	0.52743(19)	1.09191(14)	0.0406(8)
H30A_2	0.319989	0.494283	1.061828	0.061
H30B_2	0.300689	0.560432	1.100721	0.061
H30C_2	0.347079	0.493072	1.121268	0.061
C31_2	0.05232(11)	0.65420(15)	1.05410(10)	0.0208(5)
C32_2	0.02237(12)	0.72688(15)	1.05265(11)	0.0232(5)
C33_2	0.05429(12)	0.79733(15)	1.06130(11)	0.0264(6)
H33_2	0.033866	0.846701	1.060324	0.032
C34_2	0.11496(12)	0.79750(16)	1.07127(11)	0.0247(6)
C35_2	0.14395(12)	0.72464(16)	1.07282(11)	0.0247(6)
H35_2	0.185433	0.723651	1.080489	0.030

C36_2	0.11372(12)	0.65277(15)	1.06341(11)	0.0223(5)
C37_2	−0.04350(12)	0.73054(18)	1.04162(13)	0.0320(7)
H37A_2	−0.056568	0.785842	1.044528	0.048
H37B_2	−0.061086	0.697230	1.066565	0.048
H37C_2	−0.055682	0.710928	1.006580	0.048
C38_2	0.14839(14)	0.87464(16)	1.07978(13)	0.0341(7)
H38A_2	0.162701	0.891193	1.047477	0.051
H38B_2	0.181754	0.866940	1.106439	0.051
H38C_2	0.122463	0.915955	1.090968	0.051
C39_2	0.14704(12)	0.57532(16)	1.06307(12)	0.0288(6)
H39A_2	0.142019	0.552808	1.028143	0.043
H39B_2	0.131987	0.537652	1.087047	0.043
H39C_2	0.188777	0.585163	1.073800	0.043

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table S8. Anisotropic displacement parameters [Å^2] for compound **G**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1_1	0.0249(3)	0.0254(3)	0.0219(4)	−0.0002(3)	0.0047(3)	−0.0076(3)
C1_1	0.0185(12)	0.0198(12)	0.0208(14)	0.0039(10)	0.0021(10)	0.0013(9)
S2_1	0.0237(3)	0.0195(3)	0.0234(3)	−0.0020(2)	0.0045(3)	−0.0047(2)
C2_1	0.0270(14)	0.0205(13)	0.0234(15)	0.0016(10)	0.0035(11)	−0.0018(10)
S3_1	0.0249(3)	0.0229(3)	0.0307(4)	−0.0001(3)	0.0043(3)	−0.0064(3)
C3_1	0.0335(15)	0.0232(13)	0.0188(14)	−0.0007(10)	0.0023(11)	0.0023(11)
S4_1	0.0250(3)	0.0294(4)	0.0288(4)	0.0074(3)	0.0025(3)	−0.0083(3)
C4_1	0.0246(13)	0.0254(13)	0.0189(14)	0.0027(10)	0.0026(11)	0.0041(10)
S5_1	0.0304(4)	0.0275(3)	0.0305(4)	0.0032(3)	0.0030(3)	−0.0118(3)
C5_1	0.0221(13)	0.0237(13)	0.0214(14)	0.0035(10)	0.0030(11)	0.0003(10)
S6_1	0.0295(4)	0.0185(3)	0.0277(4)	−0.0024(3)	0.0001(3)	−0.0014(3)
C6_1	0.0197(12)	0.0181(12)	0.0188(13)	0.0017(9)	0.0004(10)	0.0008(9)
S7_1	0.0323(4)	0.0218(3)	0.0417(5)	−0.0043(3)	−0.0001(3)	−0.0046(3)
C7_1	0.0199(12)	0.0187(12)	0.0216(14)	0.0032(10)	0.0020(10)	−0.0012(9)
S8_1	0.0297(4)	0.0276(4)	0.0483(5)	0.0088(3)	0.0028(3)	−0.0113(3)
C8_1	0.0193(12)	0.0159(11)	0.0214(14)	0.0043(9)	0.0011(10)	0.0001(9)
C9_1	0.0196(12)	0.0182(12)	0.0201(13)	0.0008(10)	0.0035(10)	−0.0004(9)
C10_1	0.0227(13)	0.0161(11)	0.0217(14)	−0.0012(10)	0.0034(10)	−0.0014(9)
C11_1	0.0222(12)	0.0174(12)	0.0179(13)	0.0001(9)	0.0024(10)	−0.0011(9)
C12_1	0.0220(13)	0.0185(12)	0.0194(13)	−0.0010(10)	0.0013(10)	−0.0023(9)
C13_1	0.0232(13)	0.0181(12)	0.0226(14)	−0.0008(10)	0.0021(11)	−0.0040(10)
C14_1	0.0216(12)	0.0162(12)	0.0226(14)	0.0002(10)	0.0043(10)	−0.0043(9)
C15_1	0.0228(13)	0.0178(12)	0.0225(14)	−0.0012(10)	0.0045(10)	−0.0035(10)
C16_1	0.0206(12)	0.0186(12)	0.0225(14)	−0.0017(10)	0.0034(10)	−0.0030(9)
C17_1	0.0195(12)	0.0164(11)	0.0194(13)	−0.0009(9)	0.0045(10)	−0.0006(9)
C18_1	0.0192(12)	0.0166(12)	0.0232(14)	−0.0024(10)	0.0032(10)	−0.0012(9)
C19_1	0.0235(13)	0.0187(12)	0.0210(14)	−0.0007(10)	0.0055(10)	−0.0022(10)
C20_1	0.0197(12)	0.0189(12)	0.0192(13)	−0.0006(9)	0.0033(10)	−0.0005(9)
C21_1	0.0185(12)	0.0215(12)	0.0216(14)	0.0011(10)	0.0016(10)	0.0006(9)
C22_1	0.0199(12)	0.0184(12)	0.0248(14)	0.0024(10)	0.0030(10)	0.0002(9)
C23_1	0.0228(13)	0.0202(12)	0.0222(14)	−0.0008(10)	0.0041(11)	−0.0012(10)
C24_1	0.0187(12)	0.0247(13)	0.0206(14)	0.0014(10)	0.0052(10)	0.0016(10)
C25_1	0.0177(12)	0.0235(13)	0.0223(14)	0.0046(10)	0.0001(10)	0.0009(10)
C26_1	0.0168(12)	0.0214(12)	0.0245(14)	0.0030(10)	0.0031(10)	−0.0009(9)
C27_1	0.0217(13)	0.0310(14)	0.0227(15)	0.0066(11)	0.0015(11)	−0.0010(11)
C28_1	0.0219(13)	0.0374(16)	0.0239(15)	0.0060(12)	0.0056(11)	0.0013(11)

C29_1	0.0290(15)	0.0313(15)	0.0232(15)	−0.0010(11)	0.0028(12)	0.0044(11)
C30_1	0.0230(13)	0.0268(14)	0.0237(15)	0.0020(11)	0.0033(11)	0.0004(10)
C31_1	0.0228(13)	0.0181(12)	0.0215(14)	0.0042(10)	0.0030(10)	0.0000(9)
C32_1	0.0246(13)	0.0225(13)	0.0229(15)	0.0013(10)	0.0012(11)	−0.0026(10)
C33_1	0.0229(13)	0.0180(12)	0.0251(15)	0.0024(10)	−0.0002(11)	−0.0004(10)
C34_1	0.0263(13)	0.0183(12)	0.0191(14)	−0.0029(10)	0.0073(11)	−0.0046(10)
C35_1	0.0285(14)	0.0209(13)	0.0223(14)	−0.0003(10)	0.0041(11)	−0.0033(10)
C36_1	0.0298(14)	0.0243(13)	0.0246(15)	−0.0025(11)	0.0036(12)	−0.0084(11)
C37_1	0.0393(16)	0.0207(13)	0.0236(15)	−0.0025(11)	0.0087(12)	−0.0079(11)
C38_1	0.0346(15)	0.0189(12)	0.0257(15)	0.0004(11)	0.0074(12)	0.0009(11)
C39_1	0.0290(14)	0.0208(12)	0.0188(14)	−0.0020(10)	0.0070(11)	−0.0026(10)
C40_1	0.0232(13)	0.0159(11)	0.0191(13)	−0.0008(9)	0.0076(10)	−0.0033(9)
C41_1	0.0257(13)	0.0185(12)	0.0222(14)	−0.0027(10)	0.0056(11)	−0.0010(10)
C42_1	0.0302(14)	0.0164(12)	0.0232(14)	−0.0005(10)	0.0048(11)	−0.0026(10)
C43_1	0.0262(13)	0.0211(13)	0.0212(14)	−0.0047(10)	0.0067(11)	−0.0047(10)
C44_1	0.0202(13)	0.0228(13)	0.0233(14)	−0.0036(10)	0.0024(10)	−0.0006(10)
C45_1	0.0220(12)	0.0182(12)	0.0202(14)	−0.0020(10)	0.0055(10)	0.0004(9)
C46_1	0.0203(13)	0.0207(13)	0.0302(16)	0.0065(11)	0.0002(11)	−0.0014(10)
C47_1	0.0251(14)	0.0187(13)	0.0363(17)	0.0038(11)	0.0015(12)	−0.0033(10)
C48_1	0.0257(14)	0.0212(13)	0.0399(18)	0.0058(12)	−0.0002(13)	−0.0052(11)
C49_1	0.0277(15)	0.0408(17)	0.0282(16)	−0.0052(13)	0.0074(12)	−0.0130(12)
C50_1	0.0267(14)	0.0327(15)	0.0292(16)	−0.0027(12)	0.0061(12)	−0.0079(12)
C51_1	0.0262(14)	0.0350(16)	0.0309(17)	−0.0096(12)	0.0071(12)	−0.0086(12)
C52_1	0.0277(15)	0.0333(15)	0.0342(18)	−0.0037(13)	0.0071(13)	−0.0036(12)
C53_1	0.0354(16)	0.0278(15)	0.042(2)	−0.0084(13)	0.0093(14)	−0.0048(12)
C54_1	0.044(2)	0.0350(18)	0.056(2)	0.0019(16)	0.0100(17)	−0.0034(14)
C55_1	0.0275(14)	0.0237(13)	0.0271(16)	−0.0004(11)	0.0008(12)	−0.0031(11)
C56_1	0.0247(13)	0.0209(13)	0.0249(15)	0.0021(10)	0.0019(11)	−0.0021(10)
C57_1	0.0273(14)	0.0257(14)	0.0282(16)	−0.0008(11)	0.0044(12)	−0.0024(11)
C58_1	0.0245(14)	0.0267(14)	0.0336(17)	0.0001(12)	0.0046(12)	0.0038(11)
C59_1	0.0336(15)	0.0216(13)	0.0290(16)	−0.0010(11)	0.0051(12)	0.0012(11)
C60_1	0.0336(16)	0.0251(14)	0.043(2)	0.0020(13)	0.0051(14)	0.0021(12)
C61_1	0.0327(16)	0.0268(15)	0.0419(19)	0.0007(13)	−0.0015(14)	−0.0032(12)
C62_1	0.0514(19)	0.0223(14)	0.0317(18)	−0.0052(12)	0.0071(15)	−0.0122(13)
C63_1	0.0267(15)	0.0293(15)	0.0353(18)	0.0018(12)	0.0023(13)	0.0008(11)
C64_1	0.0270(14)	0.0247(14)	0.0357(18)	0.0010(12)	−0.0037(12)	0.0013(11)
C65_1	0.0273(14)	0.0253(14)	0.0345(17)	−0.0097(12)	0.0051(12)	−0.0073(11)
C66_1	0.0290(14)	0.0205(13)	0.0305(16)	−0.0029(11)	0.0028(12)	0.0026(10)
C67_1	0.0295(15)	0.0313(15)	0.0331(17)	−0.0034(12)	0.0029(13)	−0.0018(12)
C68_1	0.0291(15)	0.0348(16)	0.0297(17)	−0.0012(12)	0.0048(12)	0.0014(12)
C73_1	0.0275(15)	0.0401(17)	0.0341(18)	0.0073(13)	0.0036(13)	−0.0124(13)
C74_1	0.0300(15)	0.0323(15)	0.0285(16)	−0.0007(12)	0.0038(12)	−0.0092(12)
C75_1	0.0307(16)	0.0389(17)	0.0308(17)	−0.0039(13)	0.0046(13)	−0.0086(13)
C76_1	0.0364(17)	0.0360(17)	0.0376(19)	−0.0033(14)	0.0004(14)	−0.0064(13)
C77_1	0.053(2)	0.0416(19)	0.044(2)	−0.0097(16)	−0.0049(17)	0.0008(16)
C78_1	0.043(2)	0.070(3)	0.050(2)	−0.024(2)	−0.0106(18)	0.0059(18)
C69A_1	0.024(6)	0.032(6)	0.027(4)	0.005(4)	0.004(4)	−0.006(3)
C70A_1	0.032(4)	0.029(4)	0.035(4)	0.001(3)	0.006(3)	0.004(3)
C71A_1	0.037(3)	0.033(3)	0.037(4)	−0.006(3)	0.006(3)	0.007(2)
C72A_1	0.061(4)	0.050(4)	0.033(4)	−0.001(3)	0.003(3)	0.017(3)
C69B_1	0.013(7)	0.028(8)	0.039(6)	−0.001(6)	0.008(5)	−0.006(4)
C70B_1	0.029(5)	0.026(5)	0.046(7)	0.000(4)	0.011(4)	−0.004(4)
C71B_1	0.042(5)	0.036(5)	0.039(6)	0.000(4)	0.004(4)	0.007(4)
C72B_1	0.068(7)	0.045(6)	0.045(7)	0.006(5)	0.009(5)	−0.015(5)
S1_2	0.0223(3)	0.0273(3)	0.0223(4)	0.0029(3)	0.0036(3)	−0.0042(3)

C1_2	0.0201(12)	0.0234(13)	0.0206(14)	0.0029(10)	0.0022(10)	0.0043(10)
S2_2	0.0274(4)	0.0312(4)	0.0233(4)	−0.0002(3)	0.0048(3)	−0.0113(3)
C2_2	0.0202(12)	0.0220(12)	0.0212(14)	0.0026(10)	0.0018(10)	0.0044(10)
S3_2	0.0216(3)	0.0253(3)	0.0296(4)	0.0087(3)	0.0038(3)	−0.0020(3)
C3_2	0.0289(14)	0.0207(13)	0.0265(15)	0.0012(11)	0.0030(12)	0.0032(10)
S4_2	0.0278(3)	0.0207(3)	0.0287(4)	0.0015(3)	0.0028(3)	−0.0032(3)
C4_2	0.0377(16)	0.0221(13)	0.0245(15)	−0.0002(11)	0.0051(12)	0.0037(11)
C5_2	0.0341(16)	0.0267(14)	0.0242(15)	0.0031(11)	0.0076(12)	0.0044(11)
C6_2	0.0263(14)	0.0251(13)	0.0265(15)	0.0064(11)	0.0042(11)	0.0027(11)
C7_2	0.0192(12)	0.0236(13)	0.0186(13)	0.0045(10)	0.0025(10)	0.0009(10)
C8_2	0.0186(12)	0.0210(12)	0.0199(14)	0.0032(10)	0.0002(10)	0.0007(9)
C9_2	0.0193(12)	0.0234(13)	0.0211(14)	0.0020(10)	0.0004(10)	0.0029(10)
C10_2	0.0201(12)	0.0222(13)	0.0230(14)	0.0037(10)	0.0022(10)	0.0002(10)
C11_2	0.0185(12)	0.0238(13)	0.0272(15)	0.0036(11)	−0.0017(11)	0.0011(10)
C12_2	0.0210(13)	0.0239(13)	0.0249(15)	0.0034(11)	0.0005(11)	−0.0017(10)
C13_2	0.0230(13)	0.0210(13)	0.0212(14)	0.0004(10)	−0.0016(10)	−0.0019(10)
C14_2	0.0203(12)	0.0231(13)	0.0206(14)	0.0011(10)	0.0015(10)	−0.0021(10)
C15_2	0.0198(12)	0.0207(12)	0.0240(14)	0.0000(10)	0.0027(10)	−0.0015(10)
C16_2	0.0194(12)	0.0205(12)	0.0232(14)	0.0005(10)	0.0022(10)	−0.0027(9)
C17_2	0.0229(13)	0.0229(13)	0.0227(14)	0.0018(10)	0.0040(11)	−0.0042(10)
C18_2	0.0216(13)	0.0197(12)	0.0227(14)	0.0009(10)	0.0000(10)	−0.0011(10)
C19_2	0.0223(13)	0.0261(14)	0.0267(15)	0.0007(11)	0.0025(11)	−0.0023(10)
C20_2	0.0221(13)	0.0230(13)	0.0224(14)	0.0005(10)	0.0034(11)	0.0010(10)
C21_2	0.0235(13)	0.0241(13)	0.0263(15)	−0.0005(11)	0.0025(11)	0.0006(10)
C22_2	0.0288(15)	0.0226(13)	0.0302(16)	−0.0001(11)	0.0005(12)	−0.0010(11)
C23_2	0.0349(16)	0.0241(14)	0.0296(17)	−0.0001(11)	−0.0014(13)	0.0051(11)
C24_2	0.0317(16)	0.0349(16)	0.0370(19)	−0.0022(13)	0.0002(13)	0.0100(13)
C25_2	0.0294(14)	0.0253(14)	0.0237(15)	0.0008(11)	0.0043(12)	−0.0022(11)
C26_2	0.0259(14)	0.0270(14)	0.0215(14)	−0.0003(11)	0.0028(11)	−0.0012(11)
C27_2	0.0297(15)	0.0290(14)	0.0246(15)	0.0026(11)	0.0021(12)	−0.0001(11)
C28_2	0.0252(14)	0.0300(15)	0.0344(17)	0.0025(12)	0.0045(12)	0.0006(11)
C29_2	0.0294(16)	0.0334(16)	0.044(2)	0.0077(14)	0.0020(14)	0.0026(12)
C30_2	0.0372(18)	0.0376(17)	0.048(2)	0.0150(15)	0.0077(15)	0.0029(14)
C31_2	0.0248(13)	0.0199(12)	0.0182(13)	−0.0011(10)	0.0049(10)	−0.0049(10)
C32_2	0.0239(13)	0.0237(13)	0.0217(14)	0.0032(10)	0.0018(11)	−0.0013(10)
C33_2	0.0335(15)	0.0182(12)	0.0286(16)	0.0026(11)	0.0079(12)	−0.0001(11)
C34_2	0.0282(14)	0.0231(13)	0.0234(15)	−0.0012(11)	0.0053(11)	−0.0077(11)
C35_2	0.0241(13)	0.0267(14)	0.0235(15)	−0.0007(11)	0.0034(11)	−0.0060(11)
C36_2	0.0249(13)	0.0218(13)	0.0202(14)	0.0007(10)	0.0029(11)	−0.0023(10)
C37_2	0.0260(15)	0.0328(15)	0.0375(18)	0.0042(13)	0.0049(13)	0.0010(12)
C38_2	0.0387(17)	0.0215(14)	0.0431(19)	−0.0049(12)	0.0089(14)	−0.0097(12)
C39_2	0.0240(14)	0.0254(14)	0.0367(18)	−0.0019(12)	0.0023(12)	−0.0005(11)

Table S6. Bond lengths and angles for compound **G**.

Atom-Atom	**Length [Å]**
S1_1–C31_1	1.754(3)
S1_1–C32_1	1.754(3)
C1_1–C2_1	1.386(4)
C1_1–C6_1	1.420(3)
C1_1–C9_1	1.458(4)
S2_1–C33_1	1.745(3)
S2_1–C31_1	1.752(3)
C2_1–C3_1	1.384(4)
S3_1–C47_1	1.757(3)
S3_1–C46_1	1.758(3)
C3_1–C4_1	1.392(4)
S4_1–C46_1	1.749(3)
S4_1–C48_1	1.759(3)
C4_1–C5_1	1.387(4)
S5_1–C32_1	1.751(3)
S5_1–C49_1	1.820(3)
C5_1–C6_1	1.393(4)
S6_1–C33_1	1.762(3)
S6_1–C55_1	1.824(3)

C6_1–C7_1	1.474(4)
S7_1–C47_1	1.749(3)
S7_1–C67_1	1.819(3)
C7_1–C31_1	1.369(3)
C7_1–C8_1	1.469(3)
S8_1–C48_1	1.748(3)
S8_1–C73_1	1.818(3)
C8_1–C10_1	1.402(4)
C8_1–C9_1	1.419(3)
C9_1–C13_1	1.403(3)
C10_1–C11_1	1.380(3)
C11_1–C12_1	1.431(3)
C11_1–C14_1	1.458(4)
C12_1–C13_1	1.380(4)
C12_1–C16_1	1.485(4)
C14_1–C17_1	1.354(4)
C14_1–C15_1	1.454(3)
C15_1–C16_1	1.354(4)
C15_1–C19_1	1.458(4)
C16_1–C34_1	1.487(3)
C17_1–C18_1	1.486(3)
C17_1–C40_1	1.487(3)
C18_1–C20_1	1.385(4)
C18_1–C19_1	1.428(3)
C19_1–C23_1	1.377(3)
C20_1–C21_1	1.395(3)
C21_1–C22_1	1.424(4)
C21_1–C24_1	1.451(4)
C22_1–C23_1	1.397(4)
C22_1–C26_1	1.473(3)
C24_1–C30_1	1.391(4)
C24_1–C25_1	1.417(4)
C25_1–C27_1	1.397(4)
C25_1–C26_1	1.469(4)
C26_1–C46_1	1.366(4)
C27_1–C28_1	1.389(4)
C28_1–C29_1	1.393(4)
C29_1–C30_1	1.393(4)
C32_1–C33_1	1.342(4)
C34_1–C35_1	1.392(4)
C34_1–C39_1	1.408(4)
C35_1–C36_1	1.401(4)
C35_1–C61_1	1.503(4)
C36_1–C37_1	1.381(4)
C37_1–C38_1	1.392(4)
C37_1–C62_1	1.511(4)
C38_1–C39_1	1.391(4)
C39_1–C63_1	1.496(4)
C40_1–C45_1	1.397(4)
C40_1–C41_1	1.402(3)
C41_1–C42_1	1.391(4)
C41_1–C64_1	1.501(4)
C42_1–C43_1	1.393(4)
C43_1–C44_1	1.389(4)
C43_1–C65_1	1.502(3)

C44_1–C45_1	1.395(3)
C45_1–C66_1	1.506(3)
C47_1–C48_1	1.340(4)
C49_1–C50_1	1.517(4)
C50_1–C51_1	1.524(4)
C51_1–C52_1	1.516(4)
C52_1–C53_1	1.523(4)
C53_1–C54_1	1.526(5)
C55_1–C56_1	1.519(3)
C56_1–C57_1	1.526(4)
C57_1–C58_1	1.528(4)
C58_1–C59_1	1.521(4)
C59_1–C60_1	1.523(4)
C67_1–C68_1	1.520(4)
C68_1–C69B_1	1.45(3)
C68_1–C69A_1	1.586(16)
C73_1–C74_1	1.523(4)
C74_1–C75_1	1.515(4)
C75_1–C76_1	1.525(4)
C76_1–C77_1	1.526(5)
C77_1–C78_1	1.511(5)
C69A_1–C70A_1	1.552(19)
C70A_1–C71A_1	1.531(11)
C71A_1–C72A_1	1.510(10)
C69B_1–C70B_1	1.50(3)
C70B_1–C71B_1	1.520(16)
C71B_1–C72B_1	1.537(15)
S1_2–C11_2	1.746(3)
S1_2–C10_2	1.757(3)
C1_2–C6_2	1.396(4)
C1_2–C2_2	1.413(4)
C1_2–C7_2	1.472(4)
S2_2–C12_2	1.760(3)
S2_2–C10_2	1.761(3)
C2_2–C3_2	1.389(4)
C2_2–C9_2	1.451(4)
S3_2–C11_2	1.761(3)
S3_2–C19_2	1.817(3)
C3_2–C4_2	1.387(4)
S4_2–C12_2	1.750(3)
S4_2–C25_2	1.821(3)
C4_2–C5_2	1.391(4)
C5_2–C6_2	1.390(4)
C7_2–C10_2	1.363(4)
C7_2–C8_2	1.470(4)
C8_2–C13_2	1.410(4)
C8_2–C9_2	1.411(4)
C9_2–C18_2	1.405(4)
C11_2–C12_2	1.343(4)
C13_2–C14_2	1.380(4)
C14_2–C15_2	1.429(4)
C14_2–C17_2	1.459(4)
C15_2–C18_2	1.384(4)
C15_2–C16_2$^{\#1}$	1.482(4)
C16_2–C17_2	1.358(4)

C16_2–C31_2	1.487(3)
C17_2–C17_2[#1]	1.463(5)
C19_2–C20_2	1.527(4)
C20_2–C21_2	1.518(4)
C21_2–C22_2	1.527(4)
C22_2–C23_2	1.530(4)
C23_2–C24_2	1.526(4)
C25_2–C26_2	1.517(4)
C26_2–C27_2	1.524(4)
C27_2–C28_2	1.527(4)
C28_2–C29_2	1.522(4)
C29_2–C30_2	1.523(4)
C31_2–C32_2	1.397(4)
C31_2–C36_2	1.402(4)
C32_2–C33_2	1.394(4)
C32_2–C37_2	1.507(4)
C33_2–C34_2	1.387(4)
C34_2–C35_2	1.389(4)
C34_2–C38_2	1.507(4)
C35_2–C36_2	1.398(4)
C36_2–C39_2	1.507(4)
Atom-Atom-Atom	**Angle [°]**
C31_1–S1_1–C32_1	97.29(13)
C2_1–C1_1–C6_1	120.8(2)
C2_1–C1_1–C9_1	130.6(2)
C6_1–C1_1–C9_1	108.6(2)
C33_1–S2_1–C31_1	97.29(13)
C3_1–C2_1–C1_1	119.3(2)
C47_1–S3_1–C46_1	97.24(14)
C2_1–C3_1–C4_1	120.1(3)
C46_1–S4_1–C48_1	97.10(14)
C5_1–C4_1–C3_1	121.3(3)
C32_1–S5_1–C49_1	100.40(13)
C4_1–C5_1–C6_1	119.3(2)
C33_1–S6_1–C55_1	101.03(13)
C5_1–C6_1–C1_1	119.0(2)
C5_1–C6_1–C7_1	132.7(2)
C1_1–C6_1–C7_1	108.2(2)
C47_1–S7_1–C67_1	100.80(13)
C31_1–C7_1–C8_1	126.1(2)
C31_1–C7_1–C6_1	127.5(2)
C8_1–C7_1–C6_1	106.3(2)
C48_1–S8_1–C73_1	100.65(14)
C10_1–C8_1–C9_1	120.1(2)
C10_1–C8_1–C7_1	131.1(2)
C9_1–C8_1–C7_1	108.6(2)
C13_1–C9_1–C8_1	121.6(2)
C13_1–C9_1–C1_1	129.9(2)
C8_1–C9_1–C1_1	108.2(2)
C11_1–C10_1–C8_1	117.8(2)
C10_1–C11_1–C12_1	122.3(2)
C10_1–C11_1–C14_1	130.9(2)
C12_1–C11_1–C14_1	106.4(2)
C13_1–C12_1–C11_1	119.9(2)
C13_1–C12_1–C16_1	131.6(2)
C11_1–C12_1–C16_1	108.3(2)
C12_1–C13_1–C9_1	118.2(2)
C17_1–C14_1–C15_1	110.5(2)
C17_1–C14_1–C11_1	141.8(2)
C15_1–C14_1–C11_1	107.1(2)
C16_1–C15_1–C14_1	110.7(2)
C16_1–C15_1–C19_1	141.3(2)
C14_1–C15_1–C19_1	107.5(2)
C15_1–C16_1–C12_1	107.5(2)
C15_1–C16_1–C34_1	123.3(2)
C12_1–C16_1–C34_1	128.8(2)
C14_1–C17_1–C18_1	107.3(2)
C14_1–C17_1–C40_1	126.3(2)
C18_1–C17_1–C40_1	126.3(2)
C20_1–C18_1–C19_1	120.1(2)
C20_1–C18_1–C17_1	131.1(2)
C19_1–C18_1–C17_1	108.8(2)
C23_1–C19_1–C18_1	122.1(2)
C23_1–C19_1–C15_1	132.0(2)
C18_1–C19_1–C15_1	106.0(2)
C18_1–C20_1–C21_1	118.2(2)
C20_1–C21_1–C22_1	121.5(2)
C20_1–C21_1–C24_1	130.1(2)
C22_1–C21_1–C24_1	108.3(2)
C23_1–C22_1–C21_1	120.1(2)
C23_1–C22_1–C26_1	131.4(2)
C21_1–C22_1–C26_1	108.3(2)
C19_1–C23_1–C22_1	118.0(2)
C30_1–C24_1–C25_1	121.3(3)
C30_1–C24_1–C21_1	130.0(2)
C25_1–C24_1–C21_1	108.6(2)
C27_1–C25_1–C24_1	118.6(3)
C27_1–C25_1–C26_1	132.7(2)
C24_1–C25_1–C26_1	108.6(2)
C46_1–C26_1–C25_1	127.4(2)
C46_1–C26_1–C22_1	126.4(3)
C25_1–C26_1–C22_1	106.1(2)
C28_1–C27_1–C25_1	119.7(3)
C27_1–C28_1–C29_1	121.4(3)
C30_1–C29_1–C28_1	119.8(3)
C24_1–C30_1–C29_1	119.1(3)
C7_1–C31_1–S2_1	123.9(2)
C7_1–C31_1–S1_1	123.9(2)
S2_1–C31_1–S1_1	112.18(14)
C33_1–C32_1–S5_1	125.0(2)
C33_1–C32_1–S1_1	116.2(2)
S5_1–C32_1–S1_1	118.77(16)
C32_1–C33_1–S2_1	117.0(2)
C32_1–C33_1–S6_1	127.7(2)
S2_1–C33_1–S6_1	115.35(16)
C35_1–C34_1–C39_1	120.6(2)
C35_1–C34_1–C16_1	121.1(2)
C39_1–C34_1–C16_1	118.0(2)
C34_1–C35_1–C36_1	118.6(2)

C34_1–C35_1–C61_1	121.2(2)
C36_1–C35_1–C61_1	120.1(3)
C37_1–C36_1–C35_1	122.0(3)
C36_1–C37_1–C38_1	118.3(2)
C36_1–C37_1–C62_1	121.5(3)
C38_1–C37_1–C62_1	120.2(3)
C39_1–C38_1–C37_1	121.8(3)
C38_1–C39_1–C34_1	118.6(3)
C38_1–C39_1–C63_1	120.6(2)
C34_1–C39_1–C63_1	120.7(2)
C45_1–C40_1–C41_1	120.9(2)
C45_1–C40_1–C17_1	118.9(2)
C41_1–C40_1–C17_1	120.1(2)
C42_1–C41_1–C40_1	118.4(2)
C42_1–C41_1–C64_1	120.7(2)
C40_1–C41_1–C64_1	120.9(2)
C41_1–C42_1–C43_1	122.0(2)
C44_1–C43_1–C42_1	118.2(2)
C44_1–C43_1–C65_1	121.2(2)
C42_1–C43_1–C65_1	120.6(2)
C43_1–C44_1–C45_1	121.7(2)
C44_1–C45_1–C40_1	118.7(2)
C44_1–C45_1–C66_1	120.2(2)
C40_1–C45_1–C66_1	121.1(2)
C26_1–C46_1–S4_1	123.9(2)
C26_1–C46_1–S3_1	124.1(2)
S4_1–C46_1–S3_1	111.99(14)
C48_1–C47_1–S7_1	125.2(2)
C48_1–C47_1–S3_1	116.1(2)
S7_1–C47_1–S3_1	118.62(18)
C47_1–C48_1–S8_1	124.7(2)
C47_1–C48_1–S4_1	116.8(2)
S8_1–C48_1–S4_1	118.42(19)
C50_1–C49_1–S5_1	113.0(2)
C49_1–C50_1–C51_1	113.7(3)
C52_1–C51_1–C50_1	112.1(2)
C51_1–C52_1–C53_1	114.5(3)
C52_1–C53_1–C54_1	111.9(3)
C56_1–C55_1–S6_1	114.72(19)
C55_1–C56_1–C57_1	112.1(2)
C56_1–C57_1–C58_1	113.7(2)
C59_1–C58_1–C57_1	114.2(2)
C58_1–C59_1–C60_1	112.6(2)
C68_1–C67_1–S7_1	114.3(2)
C69B_1–C68_1–C67_1	111.9(10)
C67_1–C68_1–C69A_1	111.0(7)
C74_1–C73_1–S8_1	113.8(2)
C75_1–C74_1–C73_1	111.9(3)
C74_1–C75_1–C76_1	113.0(3)
C75_1–C76_1–C77_1	113.6(3)
C78_1–C77_1–C76_1	114.0(3)
C70A_1–C69A_1–C68_1	110.9(10)
C71A_1–C70A_1–C69A_1	112.7(7)
C72A_1–C71A_1–C70A_1	113.6(7)
C68_1–C69B_1–C70B_1	116.1(17)
C69B_1–C70B_1–C71B_1	114.7(13)
C70B_1–C71B_1–C72B_1	113.6(10)
C11_2–S1_2–C10_2	97.56(13)
C6_2–C1_2–C2_2	119.1(3)
C6_2–C1_2–C7_2	132.5(2)
C2_2–C1_2–C7_2	108.4(2)
C12_2–S2_2–C10_2	97.38(13)
C3_2–C2_2–C1_2	120.9(3)
C3_2–C2_2–C9_2	130.6(2)
C1_2–C2_2–C9_2	108.5(2)
C11_2–S3_2–C19_2	100.79(12)
C4_2–C3_2–C2_2	119.4(3)
C12_2–S4_2–C25_2	100.54(13)
C3_2–C4_2–C5_2	119.9(3)
C6_2–C5_2–C4_2	121.4(3)
C5_2–C6_2–C1_2	119.3(3)
C10_2–C7_2–C8_2	127.5(3)
C10_2–C7_2–C1_2	126.4(2)
C8_2–C7_2–C1_2	106.0(2)
C13_2–C8_2–C9_2	119.8(2)
C13_2–C8_2–C7_2	131.7(2)
C9_2–C8_2–C7_2	108.5(2)
C18_2–C9_2–C8_2	121.9(2)
C18_2–C9_2–C2_2	129.5(2)
C8_2–C9_2–C2_2	108.5(2)
C7_2–C10_2–S1_2	123.7(2)
C7_2–C10_2–S2_2	124.4(2)
S1_2–C10_2–S2_2	111.82(14)
C12_2–C11_2–S1_2	117.1(2)
C12_2–C11_2–S3_2	127.7(2)
S1_2–C11_2–S3_2	115.21(17)
C11_2–C12_2–S4_2	124.7(2)
C11_2–C12_2–S2_2	116.1(2)
S4_2–C12_2–S2_2	119.12(16)
C14_2–C13_2–C8_2	118.2(2)
C13_2–C14_2–C15_2	121.8(3)
C13_2–C14_2–C17_2	132.1(2)
C15_2–C14_2–C17_2	106.1(2)
C18_2–C15_2–C14_2	120.3(2)
C18_2–C15_2–C16_2$^{\#1}$	130.9(2)
C14_2–C15_2–C16_2$^{\#1}$	108.8(2)
C17_2–C16_2–C15_2$^{\#1}$	107.6(2)
C17_2–C16_2–C31_2	125.5(2)

C15_2$^{\#1}$–C16_2–C31_2	126.9(2)
C16_2–C17_2–C14_2	142.5(2)
C16_2–C17_2–C17_2$^{\#1}$	110.0(3)
C14_2–C17_2–C17_2$^{\#1}$	107.4(3)
C15_2–C18_2–C9_2	117.9(2)
C20_2–C19_2–S3_2	114.08(19)
C21_2–C20_2–C19_2	111.7(2)
C20_2–C21_2–C22_2	112.4(2)
C21_2–C22_2–C23_2	113.4(2)
C24_2–C23_2–C22_2	112.9(2)
C26_2–C25_2–S4_2	114.5(2)
C25_2–C26_2–C27_2	112.0(2)
C26_2–C27_2–C28_2	112.5(2)
C29_2–C28_2–C27_2	113.4(3)
C28_2–C29_2–C30_2	113.0(3)
C32_2–C31_2–C36_2	120.1(2)
C32_2–C31_2–C16_2	120.8(2)
C36_2–C31_2–C16_2	119.0(2)
C33_2–C32_2–C31_2	119.1(2)
C33_2–C32_2–C37_2	119.5(2)
C31_2–C32_2–C37_2	121.4(2)
C34_2–C33_2–C32_2	122.0(2)
C33_2–C34_2–C35_2	118.1(2)
C33_2–C34_2–C38_2	120.8(3)
C35_2–C34_2–C38_2	121.1(3)
C34_2–C35_2–C36_2	121.8(3)
C35_2–C36_2–C31_2	118.9(2)
C35_2–C36_2–C39_2	120.1(2)
C31_2–C36_2–C39_2	121.0(2)

Symmetry transformations used to generate equivalent atoms:
#1: -X, 1-Y, 2-Z;

Computations – Optimized geometries

Conpound G

Table S10. Atomic coordinates for G. Calculated at CAM-B3LYP/6-311++G(d,p) level of theory.

	Coordinates		
Atom	**x (Å)**	**y (Å)**	**z (Å)**
C	1,97609	1,990479	-2,6573
C	2,28453	2,845019	-1,4558
C	3,324625	3,765076	-1,50886
C	3,649916	4,568678	-0,42014
C	4,776678	5,561548	-0,51893
C	2,903163	4,432691	0,743655
C	1,851867	3,523587	0,837783
C	1,093096	3,375639	2,1302
C	1,542232	2,724801	-0,27014
C	0,476995	1,704886	-0,17031
C	0,64819	0,366946	-0,11804
C	-0,63431	-0,31798	-0,01951
C	-1,66469	0,708774	-0,02126
C	-0,98931	1,954889	-0,11434
C	-1,71033	3,131517	-0,15462
C	-3,10249	3,045407	-0,09082
C	-3,77516	1,810969	0,007734
C	-5,22641	2,059174	0,035677
C	-5,38412	3,525285	-0,0324
C	-4,10068	4,108349	-0,11283
C	-3,93765	5,482257	-0,19221
C	-5,0645	6,296009	-0,19031
C	-6,33385	5,732388	-0,10706
C	-6,50345	4,352895	-0,02655
C	-6,20858	1,122806	0,090313
S	-5,9062	-0,61237	0,215666
C	-7,57118	-1,14372	0,011275
S	-7,87023	-2,87914	-0,00508
C	-6,8648	-3,38375	-1,43873
C	-8,50429	-0,18356	-0,04028
S	-10,2478	-0,38992	-0,22884
C	-10,6925	-0,98238	1,434775
S	-7,93573	1,479775	0,079426
C	-3,03746	0,62226	0,044027
C	-0,46387	-1,65583	0,032945

C	-1,53031	-2,67451	0,133584
C	-2,27004	-2,79523	1,320715
C	-1,95798	-1,94209	2,522276
C	-3,31134	-3,71386	1,374975
C	-3,64035	-4,51542	0,285875
C	-4,76496	-5,5104	0,387503
C	-2,89698	-4,37801	-0,87993
C	-1,84445	-3,47043	-0,97512
C	-1,08902	-3,32057	-2,26923
C	1,002144	-1,90633	-0,02376
C	1,678277	-0,66041	-0,11675
C	3,05113	-0,57543	-0,18463
C	3,78761	-1,76494	-0,15041
C	5,238973	-2,01499	-0,18133
C	5,394715	-3,482	-0,12257
C	4,110915	-4,06332	-0,03823
C	3,946187	-5,43719	0,037257
C	5,071871	-6,25258	0,026495
C	6,341544	-5,69064	-0,06202
C	6,512741	-4,31107	-0,13871
C	6,222564	-1,08028	-0,22447
S	5,924792	0,656935	-0,32965
C	7,586319	1,182579	-0,07934
S	7,873577	2,919409	0,002628
C	6,767659	3,382446	1,375775
C	8,518153	0,22024	-0,03475
S	10,25818	0,446096	0,132606
C	10,50354	-0,19846	1,819779
S	7,948144	-1,43959	-0,23403
C	3,114076	-2,99881	-0,05317
C	1,722032	-3,0837	0,013237
H	2,511039	2,351753	-3,53585
H	0,907489	1,987594	-2,88062
H	2,269739	0,951822	-2,48778
H	3,899084	3,857568	-2,42519
H	5,687833	5,084063	-0,88678
H	4,994943	6,015137	0,448598
H	4,526079	6,364344	-1,21694
H	3,148362	5,042798	1,607079
H	1,521558	4,00667	2,908977
H	1,113035	2,339962	2,477764
H	0,042727	3,649367	2,011082

H	-1,21223	4,091353	-0,23375
H	-2,94656	5,916661	-0,2544
H	-4,9551	7,372059	-0,25158
H	-7,20711	6,37357	-0,10289
H	-7,5074	3,960514	0,041261
H	-7,06524	-4,44426	-1,58282
H	-5,80293	-3,24438	-1,2463
H	-7,17222	-2,8317	-2,32423
H	-11,7799	-1,04724	1,455144
H	-10,3582	-0,2746	2,190549
H	-10,2679	-1,96753	1,616366
H	-3,49151	-0,35359	0,114759
H	-2,25013	-0,90283	2,353703
H	-0,88899	-1,94113	2,743744
H	-2,49198	-2,30298	3,401593
H	-3,88352	-3,80711	2,292668
H	-4,50151	-6,32461	1,067438
H	-4,99941	-5,94835	-0,5834
H	-5,66971	-5,0399	0,77908
H	-3,1454	-4,98616	-1,7438
H	-1,51747	-3,95274	-3,04707
H	-0,03759	-3,59123	-2,15244
H	-1,11279	-2,28495	-2,61674
H	3,506466	0,399647	-0,25797
H	2,954791	-5,87043	0,102418
H	4,961123	-7,3287	0,083888
H	7,213688	-6,33323	-0,07482
H	7,516514	-3,91961	-0,21359
H	6,964775	4,435673	1,569971
H	7,006136	2,799392	2,262822
H	5,720789	3,260896	1,105531
H	11,57332	-0,13739	2,015713
H	10,18417	-1,23622	1,889549
H	9,965352	0,415608	2,538961
H	1,223022	-4,04319	0,090688

Conpound 10

Table S11. Atomic coordinates for 10. Calculated at CAM-B3LYP/6-311++G(d,p) level of theory.

Atom	x (Å)	y (Å)	z (Å)
O	7,934541	0,180693	0,190744
C	7,189195	-0,77086	0,102897
C	7,571905	-2,21464	0,04119
C	6,40521	-2,98255	-0,05418
C	6,483264	-4,35898	-0,12636
C	7,748647	-4,952	-0,10135
C	8,90389	-4,18527	-0,00639
C	8,82221	-2,79359	0,066377
C	5,702831	-0,75299	0,035643
C	5,239253	-2,06999	-0,05627
C	3,880808	-2,34835	-0,12906
C	4,843438	0,338421	0,054199
C	3,488953	0,070443	-0,01778
C	3,011056	-1,26895	-0,1019
C	1,52844	-1,25707	-0,16477
C	0,64238	-2,43671	-0,25833
C	0,454044	-3,25996	0,858672
C	1,161824	-2,97217	2,156392
C	-0,43161	-4,33134	0,76734
C	-1,13081	-4,60378	-0,402
C	-2,07736	-5,76984	-0,49781
C	-0,92966	-3,77117	-1,49909
C	-0,05585	-2,69196	-1,44938
C	0,122479	-1,81267	-2,65919
C	1,150402	0,036104	-0,12539
C	2,305681	0,92268	-0,03119
C	1,906337	2,212951	0,007273
C	2,741425	3,426324	0,1062
C	2,870916	4,274643	-1,00223
C	2,19229	3,949839	-2,30704
C	3,66289	5,412424	-0,88998
C	4,324311	5,730178	0,291346
C	5,20195	6,949377	0,381365
C	4,178083	4,875627	1,378693
C	3,400755	3,724294	1,306728
C	3,271873	2,824209	2,507889
C	0,417185	2,211891	-0,05153
C	-0,03937	0,872909	-0,13384

C	-1,37705	0,555029	-0,198
C	-2,30314	1,604717	-0,17185
C	-3,77522	1,608021	-0,20499
C	-4,17455	3,028327	-0,15901
C	-3,00661	3,817223	-0,07907
C	-3,07352	5,199918	-0,01473
C	-4,31946	5,815335	-0,03248
C	-5,4771	5,047958	-0,11687
C	-5,41556	3,658794	-0,18227
C	-4,5884	0,520762	-0,24037
S	-4,00384	-1,14235	-0,32593
C	-5,55603	-1,93681	-0,08326
S	-5,55056	-3,69665	0,008484
C	-4,39415	-3,96229	1,392126
C	-6,63583	-1,14334	-0,05269
S	-8,31515	-1,65677	0,098475
C	-8,68567	-1,05341	1,778018
S	-6,34887	0,587067	-0,25807
C	-1,84593	2,934818	-0,0853
C	-0,48754	3,253031	-0,02128
H	5,592204	-4,97056	-0,20115
H	7,829828	-6,03098	-0,15728
H	9,871268	-4,67163	0,010852
H	9,712652	-2,18085	0,140557
H	3,507544	-3,36316	-0,20218
H	5,225327	1,350411	0,119423
H	0,970704	-1,94843	2,486711
H	2,244256	-3,07588	2,054474
H	0,830309	-3,65262	2,940729
H	-0,58366	-4,96189	1,637387
H	-3,05498	-5,45034	-0,86615
H	-2,2175	-6,2513	0,470694
H	-1,69737	-6,52115	-1,19458
H	-1,47027	-3,96858	-2,41936
H	1,17886	-1,64703	-2,8796
H	-0,32906	-0,83019	-2,50217
H	-0,3459	-2,26123	-3,53538
H	1,105304	4,005366	-2,21733
H	2,432859	2,934947	-2,6318
H	2,502459	4,642105	-3,08976
H	3,769083	6,065347	-1,75041
H	4,867031	7,731726	-0,30146

H	6,233814	6,70127	0,116996
H	5,21232	7,35735	1,393376
H	4,681293	5,112001	2,310773
H	3,711827	3,290145	3,389739
H	3,778248	1,870243	2,342613
H	2,226079	2,59642	2,724533
H	-1,66135	-0,48346	-0,26259
H	-2,16835	5,792782	0,047029
H	-4,39048	6,895202	0,016139
H	-6,44435	5,535626	-0,1352
H	-6,33985	3,104855	-0,25414
H	-4,41116	-5,0335	1,587345
H	-4,7356	-3,42697	2,275583
H	-3,38087	-3,66537	1,129752
H	-9,73238	-1,29252	1,96211
H	-8,54631	0,023642	1,843918
H	-8,06093	-1,56443	2,507712
H	-0,15552	4,282842	0,047914

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