Supporting Information

The coordination chemistry of phosphinidene sulfides. Synthesis and catalytic properties of Pd_4 and Pt_4 clusters.

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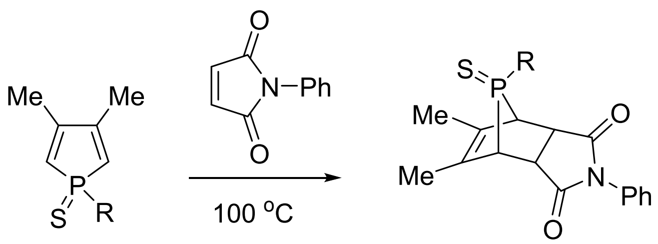
General Experimental Details

All reactions were performed under nitrogen using solvents dried by standard methods. NMR spectra were obtained using Bruker AV300 spectrometer. All spectra were recorded in $CDCl_3$. All coupling constants (*J* values) are reported in hertz (Hz). Chemical shifts are expressed in parts per million (ppm) downfield from internal TMS. HRMS spectra were obtained on an Agilent 1290-6540 UHPLC Q-Tof HR-MS spectrometer. Element analyses were performed on a Thermo Flash EA 1112 automatic element analyzer. X-ray crystallographic analyses were performed on an Oxford diffraction Gemini E diffractometer. Silica gel (200-300 mesh) was used for the chromatographic separations. 1-R-3,4-dimethylphosphole were prepared according to the literature method (R. Tian and F. Mathey, *Organometallics*, 2010, **29**, 1873). All commercially available reagents were used without further purification.

Experimental Proceduresand Characterization Data



1a R = Ph, **1b** R = 4-Tol,
1c R = 2-Th, **1d** R = 2-(1-methylpyrrolyl)

A solution of N-Phenylmaleimide (623 mg, 3.6mmol) and 1-R-3,4-dimethylphospholesulfide (3 mmol) in toluene (30 mL) was stirred at 100 °C for 3 h (^{31}P NMR: δ = 106.8 ppm for **1a,** δ = 106.8 ppm for **1b**; δ = 92.8 ppm for **1c**; δ = 90.4 ppm for **1d**). After evaporation of the solvent, the residue was chromatographed on silica gel with CH_2Cl_2 as eluent to give pure **1 a-d**

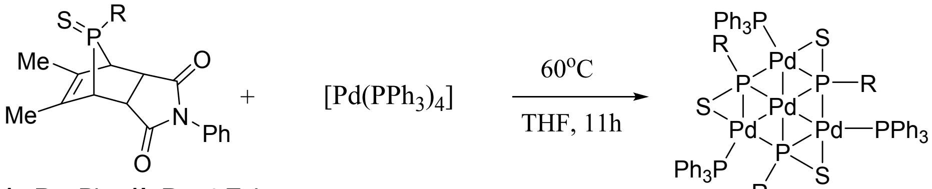
1a, yellowish solid, 1.05 g, 2.67mmol, 89%. ^{31}P NMR (121 MHz, $CDCl_3$): δ 106.8; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.63(d, *J* = 2.1 Hz, 6H), 3.55 -3.58(m, 2H), 4.31 -4.35(t, *J* = 1.2 Hz,2H), 7.06- 7.10(m, 2H), 7.37 -7.62(m, 8H); ^{13}C NMR(75 MHz, $CDCl_3$): δ 15.19(s, CH_3), 15.23(s, CH_3), 44.97(d, $_{CP}$= 18.6 Hz, CH), 52.00(d, J_{CP}= 50.9 Hz, CH), 126.39(s, CH, Ph), 128.80(s, CH, Ph), 128.94(d, J_{CP}= 2.8 Hz, CH,Ph), 129.29(s, CH, NPh), 129.89(d, J_{CP}= 13.8 Hz, CH, NPh), 130.46(d, J_{CP}= 80.4 Hz, C, Ph), 131.60(d, J_{CP}= 3.1 Hz, CH, Ph), 132.70(d, J_{CP}= 6.9 Hz, C, NPh), 175.47(d, J_{CP}= 15.4 Hz, CO). HR-MS (ESI) calcd for $C_{22}H_{20}NO_2PS$: $[M+H]^+$, 394.1025; found m/z 394.1030.

1b, yellowish solid, 952 mg, 2.33 mmol, 78%. ^{31}P NMR (121 MHz, $CDCl_3$): δ 106.8; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.63 (d, *J*= 1.8 Hz, 6H), 2.39 (s, 3H), 3.52 - 3.54 (m, 2H), 4.31 (s, 2H), 7.07 - 7.10 (m, 2H), 7.23 - 7.26 (m, 2H), 7.39 - 7.51 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 15.22 (d, J_{CP}= 3.8 Hz, Me), 21.54 (d, J_{CP}= 1.1 Hz, CH_3), 45.07 (d, J_{CP}= 18.6 Hz, CH), 52.12 (d, J_{CP}= 51.1 Hz, CH), 126.41 (s, CH, NPh), 126.82 (d, J_{CP}= 82.2 Hz, C, Ph), 128.88 (s, CH, NPh), 129.27 (s, CH, NPh), 129.59 (d, J_{CP}= 12.4 Hz, CH, Ph), 129.81 (d, J_{CP}= 45.4 Hz, CH, Ph), 131.61 (s, C, NPh), 132.61 (d, J_{CP}= 7.0 Hz, C), 142.19

(d, J_{CP}= 3.0 Hz, C, Ph), 175.53 (d, J_{CP}= 15.4 Hz, CO). HR-MS (ESI) calcd for $C_{23}H_{22}NO_2PS$: $[M+H]^+$, 408.1182; found m/z 408.1187.

1c, yellowish solid, 622.4 mg, 1.6 mmol, 52%. ^{31}P NMR (121 MHz, $CDCl_3$): δ 92.8; ^1H NMR (300 MHz, $CDCl_3$) δ 1.83 (d, J = 1.8 Hz, 6H), 3.33 - 3.35 (m, 2H), 4.18 (d, J = 0.9 Hz, 2H), 7.03 - 7.05 (m, 2H), 7.12 - 7.19 (m, 1H), 7.36 - 7.43 (m, 3H), 7.96 - 7.63 (m, 1H), 8.05 - 8.09 (m, 1H) ; ^{13}C NMR (75 MHz, $CDCl_3$): δ 15.91 (d, J_{CP}= 3.8 Hz, Me), 44.97 (d, J_{CP}= 19.7 Hz, CH), 53.94 (d, J_{CP}=56.1 Hz, CH), 123.16 (d, J_{CP}= 79.9 Hz, C, Th), 126.41 (s, CH, NPh), 128.00 (d, J_{CP}= 16.4 Hz, CH, Th), 128.96 (s, CH, NPh), 129.32 (s, CH, NPh), 131.57 (s, C, NPh), 133.89 (d, J_{CP}= 5.9 Hz, C), 135.67 (s, CH, Th), 144.33 (d, J_{CP}= 13.9 Hz, CH, Th), 175.34 (d, J_{CP}= 16.6 Hz, CO). HR-MS (ESI) calcd for $C_{20}H_{18}NO_2PS_2$: $[M+H]^+$, 400.0593; found m/z 400.0589.

1d, yellowish solid, 760.3 mg, 1.9 mmol, 64%. ^{31}P NMR (121 MHz, $CDCl_3$): δ 90.4; ^1H NMR (300MHz, $CDCl_3$) δ 1.70 (d, J = 2.1 Hz, 6H), 3.50 - 3.52 (m, 2H), 3.89 (s, 3H), 4.28 - 4.29 (t, 2H), 6.12 - 6.15 (m, 1H), 6.40 - 6.43 (m, 1H), 6.82 - 6.85 (m, 1H), 7.07 - 7.10 (m, 2H), 7.37 - 7.48 (m, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$): δ 15.26 (d, J_{CP}= 3.8 Hz, Me), 36.16 (d, J_{CP}= 2.6 Hz, CH_3), 44.81 (d, J_{CP}= 20.2 Hz, CH), 53.04 (d, J_{CP}= 54.3 Hz, CH), 108.73 (d, J_{CP}= 11.4 Hz, CH, Py), 117.47 (d, J_{CP}= 104.3 Hz, C, Py), 118.37 (d, J_{CP}= 12.3 Hz, CH, Py), 126.38 (s, CH, NPh), 128.88 (s, CH, NPh), 129.27 (s, CH, NPh), 129.33 (s, CH, Py), 131.56 (s, C, NPh), 132.24 (d, J_{CP}= 6.9 Hz, C), 175.46 (d, J_{CP}= 16.1 Hz, CO). HR-MS (ESI) calcd for $C_{10}H_{11}PS$: $[M+H]^+$, 397.1134; found m/z 397.1142.



1a R = Ph, **1b** R = 4-Tol,
1c R = 2-Th, **1d** R = 2-(1-methylpyrrolyl)

2a, **2b**, **2c**, **2d**

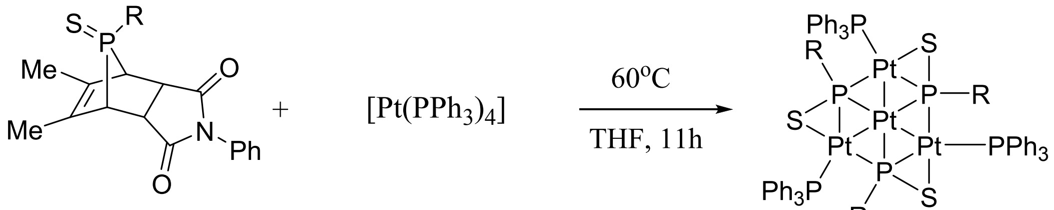
Tetrakis(triphenylphosphine)palladium(1.39 g, 1.2mmol) was added to a solution of **1 a-d**(0.9 mmol) in THF (10 mL) at 60 °C and stirred for 11 h in an 50mL-Schlenk flask. After evaporation of the solvent, the residue was chromatographed on silica gel with petroleum ether/CH_2Cl_2 (2:1) as eluent to give pure **2 a-d.** Single Crystal for X-ray analysis was grown from a solution of the compound **2** in dichloromethane/ethyl acetate.

2a, wine red solid，283.6 mg, 0.17 mmol, 58%. ^{31}P NMR (121 MHz, $CDCl_3$): δ 25.2 (q, J_{PP}= 26.1 Hz), 229.2 (q, J_{PP}= 23.8 Hz); ^1H NMR (300 MHz, $CDCl_3$) δ 6.53 (bs, 6H), 6.62 (t, J = 7.5 Hz, 6H), 6.89 (t, J = 6.9 Hz, 3H), 7.20-7.38 (m, 27H), 7.50 - 7.55 (t, J = 8.1 Hz, 18H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 126.80 (bs, CH, Ph), 128.16 (d, J = 7.8 Hz, CH, PPh_3), 129.57 (s, CH, PPh_3), 131.17 (bs, CH, Ph), 134.02 (d, J_{CP}= 13.1 Hz, CH, PPh_3), 134.81 (d, J_{CP}= 40.7 Hz, C, PPh_3), 145.07 (s, C, Ph). Elemental analysis calcd (%) for $C_{72}H_{60}P_6Pd_4S_3$: C 52.96, H 3.70; found C 52.46, H 3.61.

2b, wine red solid, 270.8 mg, 0.16 mmol, 54%. ^{31}P NMR (121 MHz, $CDCl_3$): δ 24.9 (q, J_{PP}= 27.6 Hz), 230.4 (q, J_{PP}= 23.0 Hz); ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.12 (s, 9H), 6.47 (s, 12H, Ph), 7.22 - 7.34 (m, 27H), 7.49 - 7.55(mt, 18H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.15 (s, CH, Me), 127.51 (s, CH, Ph), 128.12 (d, J = 7.2 Hz, CH, PPh_3), 129.49 (s, CH, PPh_3), 131.18 (bs, CH, Ph), 134.05 (d, J = 12.4 Hz, CH, PPh_3), 134.90 (d, J_{CP}= 38.5 Hz, C, PPh_3), 138.21 (s, C,Ph), 142.28 (s, C, Ph). Elemental analysis calcd (%) for $C_{75}H_{66}P_6Pd_4S_3$: C 53.78, H 3.97; found C 53.36, H 4.10.

2c, wine red solid, 237.3 mg, 0.14 mmol, 48%.^{31}P NMR (121 MHz, $CDCl_3$): δ 25.2 (q, J_{PP}= 26.7 Hz), 206.8 (q, J_{PP}= 25.3 Hz); ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.06 (bs, 3H), 6.49 (t, J = 6.0 Hz 3H), 7.17 - 7.61 (m, 48H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 127.42 (bs, CH, Th), 128.22 (d, J = 9.8 Hz, CH, Ph), 129.64 (s, CH, Ph), 131.33 (s, CH, Th), 132.38 (s, C Th), 134.14 (d, J_{CP}= 23.4 Hz, CH, Ph), 134.55 (d, J_{CP}= 38.5 Hz, C, Ph). Elemental analysis calcd (%) for $C_{66}H_{54}P_6Pd_4S_6$: C 48.01, H 3.30; found C 47.78, H 3.49.

2d, wine red solid, 204.6 mg, 0.13 mmol, 42%.^{31}P NMR (121 MHz, $CDCl_3$): δ 27.1 (q, J_{PP}= 26.2 Hz), 195.1 (q, J_{PP}= 24.8 Hz); ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.05 (s, 3H, Me), 5.82-5.84 (m, 3H), 6.10(bs, 3H), 6.60 (t, J = 1.8 Hz 3H), 7.25 - 7.62 (m, 45H, Ph); ^{13}C NMR (75 MHz, $CDCl_3$): δ 34.01(s, Me), 127.50 (s, CH), 128.17 (d, J = 9.8 Hz, CH, Ph), 128.18 (d, J = 3.2 Hz, CH), 129.52 (s, CH, Ph), 133.92 (d, J_{CP}= 14.0 Hz, CH, Ph), 133.92 (d, J_{CP}= 3.8 Hz, CH), 134.59 (d, J_{CP}= 37.3 Hz, CH, Ph), 135.99 (s, C). Elemental analysis calcd (%) for $C_{68}H_{60}N_3P_6Pd_4S_3$: C 50.20, H 3.72; found C 50.14, H 3.89.



1a R = Ph, **1b** R = 4-Tol,
1d R = 2-(1-methylpyrrolyl)

4a, **4b**, **4d**

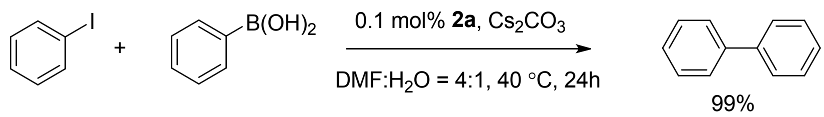
Tetrakis(triphenylphosphine)platinum (497.7 mg, 0.4 mmol for **2a**; 995.4 mg, 0.8 mmol for **2b** and **2d**) was added to a solution of **1**(117.9 mg, 0.3 mmol for **1a**; 244.2 mg, 0.6 mmol for **1b**; 237.6 mg, 0.6 mmol for **1d**) in THF (10 mL) at 60 °C and stirred for 11 h. After evaporation of the solvent, the residue was chromatographed on silica gel with petroleum ether/CH_2Cl_2 (2:1) as eluent to give pure **4a, 4b** and **4d**. Single Crystal for X-ray analysis was grown from a solution of the compound **4a** in dichloromethane/ethyl acetate.

4a, yellow solid，99.3 mg, 0.05 mmol, 51%. ^{31}P NMR (121 MHz, $CDCl_3$): δ 19.5 (q, J_{PP}= 28.3 Hz, J_{PPt}= 5326.7 Hz), 165.3 (q, J_{PP}= 28.2 Hz ,J_{PPt}= 3893.2 Hz, J_{PPt}= 1757.1 Hz); ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.61 - 6.65 (m, 12H), 6.83 - 6.84 (m, 3H), 7.28 - 7.35 (m, 27H), 7.55 - 7.61 (m, 18H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 126.49 (d, J = 11.2 Hz, CH, Ph), 128.03 (d, J = 10.8 Hz, CH, PPh_3), 129.92 (s, CH, PPh_3), 131.87 (d, J = 15.6 Hz, CH, Ph), 133.97 (d, J = 12.5 Hz, CH, PPh_3), 134.61 (d, J = 53.6 Hz C, PPh_3). Elemental analysis calcd (%) for $C_{72}H_{60}P_6Pt_4S_3$: C: 43.51, H 3.04; found C: 43.14, H: 3.43.

4b, yellow solid，202.8 mg, 0.1 mmol, 49%. ^{31}P NMR (121 MHz, $CDCl_3$): δ 19.4 (q, J_{PP}= 28.7 Hz, J_{PPt}= 5328.5 Hz), 166.1 (q, J_{PP}= 29.0 Hz, J_{PPt}= 3857.6 Hz, J_{PPt}= 1714.0 Hz); ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.11 (s, 9H), 6.46 - 6.64 (m, 12H), 7.23 - 7.33 (m, 27H), 7.55 - 7.61 (m, 18H); ^{13}C NMR (75 MHz,

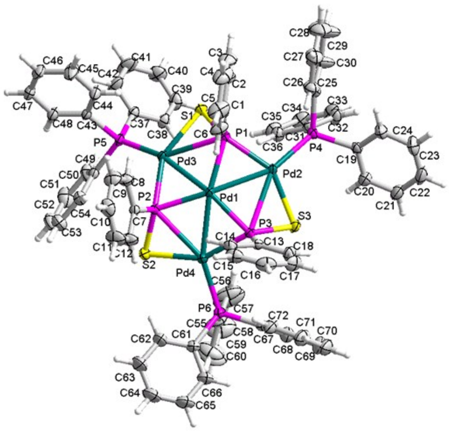
$CDCl_3$): δ 21.11(s, CH, Me), 127.30 (d, *J* = 11.8 Hz, CH, Ph), 128.01 (d, *J* = 10.7 Hz, CH, PPh_3), 129.88 (s, CH, PPh_3), 131.81-132.03 (bs, CH, Ph), 133.73 (s, C, Ph), 134.02 (d, *J* = 12.4 Hz, CH, PPh_3), 134.70 (d, *J* = 54.2 Hz, C, PPh_3), 138.07 (s, C, Ph). Elemental analysis calcd (%) for $C_{75}H_{66}P_6Pt_4S_3$: C: 44.38, H: 3.28; found C: 44.39, H: 3.49.

4d, yellow solid，170.3 mg, 0.09 mmol, 43%. ^{31}P NMR (121 MHz, $CDCl_3$): δ 22.0 (q, J_{PP}= 29.4 Hz, J_{PPt}= 5307.8 Hz), 132.2 (q, J_{PP}= 29.3 Hz, J_{PPt}= 3847.8 Hz, J_{PPt}= 1731.6 Hz); ^1H NMR (300 MHz, $CDCl_3$) δ 2.10 (s, 9H), 5.81 (bs, 3H), 6.08 (bs, 3H), 6.65 (bs, 3H), 7.24 - 7.31 (m, 27H), 7.58 - 7.64 (m, 18H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 33.76 (s, CH, Me), 106.86 (s, CH, Py), 118.45 (s, CH, Py), 128.08 (d, *J* = 10.7 Hz, CH, PPh_3), 129.91 (s, CH, PPh_3), 133.60 (s, C, Py), 133.86 (d, *J* = 12.5 Hz, C, PPh_3), 134.42 (d, *J* = 53.6 Hz, C, PPh_3). Elemental analysis calcd (%) for $C_{68}H_{60}P_6\ N_3Pt_4S_3$: C 41.22, H 3.05; found C 41.13, H 3.18.



A solution of iodobenzene (2 mmol, 223 µL), phenylboronic acid (3 mmol, 366 mg), Pd cluster **2a** (0. 002 mmol, 3.3 mg) and Cs_2CO_3 (6 mmol, 1.95 g) in 5 mL DMF/H_2O (4/1) mixture was stirred at 40 ^oC for 24h. The organic components were extracted with CH_2Cl_2×3. Combined the organic phase and the solvent was removed under vacuum. The residue was chromatographed on silica gel with petroleum ether as eluent to give pure biphenyl (306 mg, 1.98 mmol, 99%).

X-Ray Diffraction Data



2a

Table 1 Crystal data and structure refinement for 2a.

Empirical formula	$C_{72}H_{60}P_6Pd_4S_3$
Formula weight	1632.80
Temperature/K	293(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	32.9703(4)
b/Å	15.48579(16)
c/Å	29.9766(4)
α/°	90.00
β/°	93.7902(11)
γ/°	90.00
Volume/Å^3	15271.7(3)
Z	8
ρ_{calc}g/cm^3	1.420
μ/mm^{-1}	1.171
F(000)	6512.0
Crystal size/mm^3	0.25 × 0.19 × 0.18
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.9 to 52.74
Index ranges	-41 ≤ h ≤ 39, -19 ≤ k ≤ 18, -37 ≤ l ≤ 33
Reflections collected	72647
Independent reflections	15598 [R_{int} = 0.0528, R_{sigma} = 0.0424]
Data/restraints/parameters	15598/0/766

Goodness-of-fit on F^2	1.004
Final R indexes [I>=2σ (I)]	R_1 = 0.0341, wR_2 = 0.0812
Final R indexes [all data]	R_1 = 0.0471, wR_2 = 0.0855
Largest diff. peak/hole / e Å^{-3}	0.61/-0.58

Table 2 Bond Lengths for 2a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.396(5)	C45	C46	1.358(6)
C1	C6	1.379(5)	C46	C47	1.349(6)
C1	P1	1.810(4)	C47	C48	1.383(5)
C2	C3	1.384(6)	C49	C50	1.390(5)
C3	C4	1.381(7)	C49	C54	1.391(5)
C4	C5	1.358(7)	C49	P5	1.827(4)
C5	C6	1.397(6)	C50	C51	1.392(6)
C7	C8	1.381(5)	C51	C52	1.367(8)
C7	C12	1.377(5)	C52	C53	1.389(8)
C7	P2	1.823(3)	C53	C54	1.392(6)
C8	C9	1.375(6)	C55	C56	1.368(7)
C9	C10	1.359(6)	C55	C60	1.382(7)
C10	C11	1.354(6)	C55	P6	1.819(4)
C11	C12	1.375(6)	C56	C57	1.386(7)
C13	C14	1.382(5)	C57	C58	1.332(10)
C13	C18	1.375(4)	C58	C59	1.350(10)
C13	P3	1.822(3)	C59	C60	1.382(9)
C14	C15	1.378(5)	C61	C62	1.361(6)
C15	C16	1.369(6)	C61	C66	1.367(5)
C16	C17	1.366(6)	C61	P6	1.838(4)
C17	C18	1.386(5)	C62	C63	1.372(7)
C19	C20	1.388(5)	C63	C64	1.339(7)
C19	C24	1.388(5)	C64	C65	1.358(7)
C19	P4	1.830(3)	C65	C66	1.373(6)
C20	C21	1.379(5)	C67	C68	1.385(5)
C21	C22	1.366(7)	C67	C72	1.367(5)
C22	C23	1.353(7)	C67	P6	1.832(3)
C23	C24	1.394(6)	C68	C69	1.404(6)
C25	C26	1.396(6)	C69	C70	1.357(7)
C25	C30	1.350(6)	C70	C71	1.376(7)
C25	P4	1.821(4)	C71	C72	1.381(6)
C26	C27	1.378(6)	P1	Pd1	2.2731(8)

C27	C28	1.332(8)	P1	Pd2	2.2806(8)
C28	C29	1.343(10)	P1	Pd3	2.8057(8)
C29	C30	1.402(8)	P1	S1	2.0212(12)
C31	C32	1.386(5)	P2	Pd1	2.2944(8)
C31	C36	1.392(5)	P2	Pd3	2.2905(8)
C31	P4	1.825(4)	P2	Pd4	2.7056(8)
C32	C33	1.382(6)	P2	S2	2.0228(12)
C33	C34	1.364(6)	P3	Pd1	2.2829(7)
C34	C35	1.368(6)	P3	Pd2	2.7405(8)
C35	C36	1.384(5)	P3	Pd4	2.2770(8)
C37	C38	1.386(5)	P3	S3	2.0151(11)
C37	C42	1.386(5)	P4	Pd2	2.2865(8)
C37	P5	1.827(3)	P5	Pd3	2.2971(8)
C38	C39	1.369(5)	P6	Pd4	2.2946(9)
C39	C40	1.374(6)	Pd1	Pd2	2.6559(3)
C40	C41	1.367(6)	Pd1	Pd3	2.6517(3)
C41	C42	1.374(6)	Pd1	Pd4	2.6768(3)
C43	C44	1.370(5)	Pd2	S3	2.4121(8)
C43	C48	1.390(4)	Pd3	S1	2.3984(9)
C43	P5	1.823(3)	Pd4	S2	2.4166(8)
C44	C45	1.397(5)			

Table 3 Bond Angles for 2a.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	P1	121.2(3)	C1	P1	Pd1	115.99(12)
C6	C1	C2	118.3(4)	C1	P1	Pd2	115.31(11)
C6	C1	P1	120.5(3)	C1	P1	Pd3	116.61(11)
C3	C2	C1	120.5(5)	C1	P1	S1	108.08(12)
C4	C3	C2	120.6(5)	Pd1	P1	Pd2	71.36(2)
C5	C4	C3	119.3(5)	Pd1	P1	Pd3	61.90(2)
C4	C5	C6	120.9(5)	Pd2	P1	Pd3	120.86(3)
C1	C6	C5	120.5(4)	S1	P1	Pd1	115.36(5)
C8	C7	P2	118.6(3)	S1	P1	Pd2	126.62(5)
C12	C7	C8	117.4(3)	S1	P1	Pd3	56.83(3)
C12	C7	P2	123.8(3)	C7	P2	Pd1	105.25(10)
C9	C8	C7	121.3(4)	C7	P2	Pd3	115.02(11)
C10	C9	C8	120.0(4)	C7	P2	Pd4	109.96(10)
C11	C10	C9	119.9(4)	C7	P2	S2	108.23(11)
C10	C11	C12	120.4(4)	Pd1	P2	Pd4	64.120(19)

C7	C12	C11	121.0(4)	Pd3	P2	Pd1	70.67(2)
C14	C13	P3	117.8(2)	Pd3	P2	Pd4	122.37(3)
C18	C13	C14	118.7(3)	S2	P2	Pd1	121.05(4)
C18	C13	P3	123.4(3)	S2	P2	Pd3	129.79(5)
C15	C14	C13	120.5(4)	S2	P2	Pd4	59.40(3)
C16	C15	C14	120.3(4)	C13	P3	Pd1	114.85(10)
C17	C16	C15	119.8(4)	C13	P3	Pd2	114.64(10)
C16	C17	C18	120.2(4)	C13	P3	Pd4	112.69(10)
C13	C18	C17	120.5(4)	C13	P3	S3	108.65(11)
C20	C19	C24	118.5(3)	Pd1	P3	Pd2	63.07(2)
C20	C19	P4	117.3(3)	Pd4	P3	Pd1	71.89(2)
C24	C19	P4	124.1(3)	Pd4	P3	Pd2	124.48(3)
C21	C20	C19	120.6(4)	S3	P3	Pd1	117.27(4)
C22	C21	C20	120.4(4)	S3	P3	Pd2	58.61(3)
C23	C22	C21	119.7(4)	S3	P3	Pd4	127.36(5)
C22	C23	C24	121.2(5)	C19	P4	Pd2	115.82(11)
C19	C24	C23	119.5(4)	C25	P4	C19	103.01(16)
C26	C25	P4	118.4(3)	C25	P4	C31	105.63(17)
C30	C25	C26	117.6(4)	C25	P4	Pd2	116.77(12)
C30	C25	P4	123.9(4)	C31	P4	C19	102.85(15)
C27	C26	C25	121.3(4)	C31	P4	Pd2	111.31(12)
C28	C27	C26	119.6(6)	C37	P5	C49	104.00(17)
C27	C28	C29	120.8(6)	C37	P5	Pd3	113.37(11)
C28	C29	C30	120.4(6)	C43	P5	C37	102.88(15)
C25	C30	C29	120.2(6)	C43	P5	C49	101.37(15)
C32	C31	C36	118.8(3)	C43	P5	Pd3	114.56(12)
C32	C31	P4	122.4(3)	C49	P5	Pd3	118.71(11)
C36	C31	P4	118.8(3)	C55	P6	C61	104.9(2)
C33	C32	C31	120.1(4)	C55	P6	C67	103.27(18)
C34	C33	C32	120.3(4)	C55	P6	Pd4	111.91(14)
C33	C34	C35	120.7(4)	C61	P6	Pd4	114.84(13)
C34	C35	C36	119.7(4)	C67	P6	C61	102.03(17)
C35	C36	C31	120.4(4)	C67	P6	Pd4	118.31(12)
C38	C37	C42	117.6(3)	P1	Pd1	P2	121.54(3)
C38	C37	P5	119.2(2)	P1	Pd1	P3	119.92(3)
C42	C37	P5	123.2(3)	P1	Pd1	Pd2	54.45(2)
C39	C38	C37	121.0(3)	P1	Pd1	Pd3	68.97(2)
C38	C39	C40	120.6(4)	P1	Pd1	Pd4	161.79(3)
C41	C40	C39	119.3(4)	P2	Pd1	Pd2	161.20(2)
C40	C41	C42	120.4(4)	P2	Pd1	Pd3	54.60(2)

C41	C42	C37	121.1(4)	P2	Pd1	Pd4	65.42(2)
C44	C43	C48	118.0(3)	P3	Pd1	P2	118.15(3)
C44	C43	P5	119.2(2)	P3	Pd1	Pd2	66.91(2)
C48	C43	P5	122.7(3)	P3	Pd1	Pd3	157.68(2)
C43	C44	C45	120.6(4)	P3	Pd1	Pd4	53.95(2)
C46	C45	C44	119.7(4)	Pd2	Pd1	Pd4	112.933(11)
C47	C46	C45	120.9(4)	Pd3	Pd1	Pd2	113.212(11)
C46	C47	C48	119.8(4)	Pd3	Pd1	Pd4	110.650(11)
C47	C48	C43	120.9(4)	P1	Pd2	P3	103.15(3)
C50	C49	P5	122.8(3)	P1	Pd2	P4	105.09(3)
C54	C49	C50	119.3(4)	P1	Pd2	Pd1	54.19(2)
C54	C49	P5	117.8(3)	P1	Pd2	S3	146.81(3)
C51	C50	C49	120.3(5)	P4	Pd2	P3	151.67(3)
C52	C51	C50	120.1(5)	P4	Pd2	Pd1	156.17(2)
C51	C52	C53	120.4(5)	P4	Pd2	S3	106.37(3)
C52	C53	C54	119.8(5)	Pd1	Pd2	P3	50.022(16)
C49	C54	C53	120.0(4)	S3	Pd2	P3	45.49(3)
C56	C55	C60	119.1(5)	S3	Pd2	Pd1	92.76(2)
C56	C55	P6	117.8(4)	P2	Pd3	P1	102.44(3)
C60	C55	P6	123.0(4)	P2	Pd3	P5	112.79(3)
C55	C56	C57	120.5(6)	P2	Pd3	Pd1	54.73(2)
C58	C57	C56	119.3(7)	P2	Pd3	S1	146.54(3)
C57	C58	C59	121.7(7)	P5	Pd3	P1	144.76(3)
C58	C59	C60	120.1(7)	P5	Pd3	Pd1	163.09(3)
C55	C60	C59	119.1(7)	P5	Pd3	S1	100.08(3)
C62	C61	C66	117.1(4)	Pd1	Pd3	P1	49.131(17)
C62	C61	P6	119.0(3)	S1	Pd3	P1	44.86(3)
C66	C61	P6	124.0(3)	S1	Pd3	Pd1	91.82(2)
C61	C62	C63	121.2(4)	P3	Pd4	P2	103.68(3)
C64	C63	C62	121.0(5)	P3	Pd4	P6	104.64(3)
C63	C64	C65	119.3(5)	P3	Pd4	Pd1	54.15(2)
C64	C65	C66	119.8(5)	P3	Pd4	S2	149.20(3)
C61	C66	C65	121.7(4)	P6	Pd4	P2	151.68(3)
C68	C67	P6	122.5(3)	P6	Pd4	Pd1	156.96(2)
C72	C67	C68	118.6(4)	P6	Pd4	S2	105.75(3)
C72	C67	P6	118.8(3)	Pd1	Pd4	P2	50.461(18)
C67	C68	C69	119.5(5)	S2	Pd4	P2	46.09(3)
C70	C69	C68	120.6(5)	S2	Pd4	Pd1	95.05(2)
C69	C70	C71	119.9(5)	P1	S1	Pd3	78.30(4)
C70	C71	C72	119.4(5)	P2	S2	Pd4	74.51(3)

C67	C72	C71	121.8(4)	P3	S3	Pd2	75.90(3)

Table 4 Torsion Angles for 2a.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	-1.5(7)	C67	C68	C69	C70	1.1(7)
C1	P1	Pd1	P2	92.36(12)	C67	P6	Pd4	P2	-172.97(15)
C1	P1	Pd1	P3	-95.01(12)	C67	P6	Pd4	P3	6.67(15)
C1	P1	Pd1	Pd2	-109.72(12)	C67	P6	Pd4	Pd1	27.91(18)
C1	P1	Pd1	Pd3	107.74(12)	C67	P6	Pd4	S2	-178.37(15)
C1	P1	Pd1	Pd4	-159.96(12)	C68	C67	C72	C71	-2.6(6)
C1	P1	Pd2	P3	99.76(14)	C68	C67	P6	C55	6.6(4)
C1	P1	Pd2	P4	-82.56(14)	C68	C67	P6	C61	115.3(3)
C1	P1	Pd2	Pd1	110.61(14)	C68	C67	P6	Pd4	-117.7(3)
C1	P1	Pd2	S3	116.41(14)	C68	C69	C70	C71	-2.4(8)
C1	P1	Pd3	P2	-93.34(13)	C69	C70	C71	C72	1.1(7)
C1	P1	Pd3	P5	87.80(14)	C70	C71	C72	C67	1.4(7)
C1	P1	Pd3	Pd1	-106.74(13)	C72	C67	C68	C69	1.3(6)
C1	P1	Pd3	S1	95.00(14)	C72	C67	P6	C55	-173.5(3)
C1	P1	S1	Pd3	-110.46(12)	C72	C67	P6	C61	-64.8(3)
C2	C1	C6	C5	1.3(6)	C72	C67	P6	Pd4	62.2(3)
C2	C1	P1	Pd1	-171.1(3)	P1	C1	C2	C3	-176.4(3)
C2	C1	P1	Pd2	108.3(3)	P1	C1	C6	C5	177.9(4)
C2	C1	P1	Pd3	-101.1(3)	P1	Pd1	Pd2	P3	166.16(4)
C2	C1	P1	S1	-39.8(3)	P1	Pd	Pd	P4	-33.00(7)

						1	2		
C2	C3	C4	C5	1.5(8)	P1	Pd1	Pd2	S3	-176.82(4)
C3	C4	C5	C6	-0.1(8)	P1	Pd1	Pd3	P2	-163.90(4)
C4	C5	C6	C1	-1.3(8)	P1	Pd1	Pd3	P5	150.13(9)
C6	C1	C2	C3	0.1(6)	P1	Pd1	Pd3	S1	15.16(3)
C6	C1	P1	Pd1	12.4(3)	P1	Pd1	Pd4	P2	-116.75(8)
C6	C1	P1	Pd2	-68.2(3)	P1	Pd1	Pd4	P3	76.20(8)
C6	C1	P1	Pd3	82.4(3)	P1	Pd1	Pd4	P6	50.59(11)
C6	C1	P1	S1	143.7(3)	P1	Pd1	Pd4	S2	-104.09(8)
C7	C8	C9	C10	1.7(7)	P1	Pd2	S3	P3	-23.04(8)
C7	P2	Pd1	P1	-93.98(11)	P2	C7	C8	C9	-176.6(3)
C7	P2	Pd1	P3	93.27(11)	P2	C7	C12	C11	175.9(4)
C7	P2	Pd1	Pd2	-165.68(11)	P2	Pd1	Pd2	P1	84.02(7)
C7	P2	Pd1	Pd3	-111.65(11)	P2	Pd1	Pd2	P3	-109.83(7)
C7	P2	Pd1	Pd4	105.13(11)	P2	Pd1	Pd2	P4	51.02(10)
C7	P2	Pd3	P1	85.87(11)	P2	Pd1	Pd2	S3	-92.81(7)
C7	P2	Pd3	P5	-94.84(11)	P2	Pd1	Pd3	P1	163.90(4)
C7	P2	Pd3	Pd1	98.27(11)	P2	Pd1	Pd3	P5	-45.97(9)
C7	P2	Pd3	S1	96.57(12)	P2	Pd1	Pd3	S1	179.06(4)
C7	P2	Pd4	P3	-86.97(11)	P2	Pd1	Pd4	P3	-167.05(4)
C7	P2	Pd4	P6	92.67(13)	P2	Pd1	Pd4	P6	167.34(7)
C7	P2	Pd	Pd	-97.75(11)	P2	Pd	Pd	S2	12.66(3)

		4	1			1	4		
C7	P2	Pd4	S2	99.89(12)	P2	Pd3	S1	P1	-14.89(8)
C7	P2	S2	Pd4	-102.88(11)	P3	C13	C14	C15	177.0(3)
C8	C7	C12	C11	1.1(6)	P3	C13	C18	C17	-177.2(3)
C8	C7	P2	Pd1	73.8(3)	P3	Pd1	Pd2	P1	-166.16(4)
C8	C7	P2	Pd3	-1.7(3)	P3	Pd1	Pd2	P4	160.85(7)
C8	C7	P2	Pd4	141.3(3)	P3	Pd1	Pd2	S3	17.02(3)
C8	C7	P2	S2	-155.5(3)	P3	Pd1	Pd3	P1	-118.05(7)
C8	C9	C10	C11	-1.5(7)	P3	Pd1	Pd3	P2	78.04(7)
C9	C10	C11	C12	1.1(8)	P3	Pd1	Pd3	P5	32.07(11)
C10	C11	C12	C7	-0.9(8)	P3	Pd1	Pd3	S1	-102.90(7)
C12	C7	C8	C9	-1.5(6)	P3	Pd1	Pd4	P2	167.05(4)
C12	C7	P2	Pd1	-101.0(3)	P3	Pd1	Pd4	P6	-25.61(7)
C12	C7	P2	Pd3	-176.4(3)	P3	Pd1	Pd4	S2	179.71(4)
C12	C7	P2	Pd4	-33.5(3)	P3	Pd4	S2	P2	-13.12(8)
C12	C7	P2	S2	29.8(3)	P4	C19	C20	C21	-177.5(3)
C13	C14	C15	C16	0.4(6)	P4	C19	C24	C23	176.4(3)
C13	P3	Pd1	P1	93.28(12)	P4	C25	C26	C27	175.3(3)
C13	P3	Pd1	P2	-93.85(12)	P4	C25	C30	C29	-174.3(6)
C13	P3	Pd1	Pd2	106.26(11)	P4	C31	C32	C33	179.3(3)
C13	P3	Pd1	Pd3	-158.59(11)	P4	C31	C36	C35	-179.4(3)
C13	P3	Pd1	Pd4	-107.21(11)	P4	Pd2	S3	P3	176.06(4)
C13	P3	Pd2	P1	-95.10(11)	P5	C37	C38	C39	-179.8(3)

C13	P3	Pd2	P4	89.63(13)	P5	C37	C42	C41	179.1(4)
C13	P3	Pd2	Pd1	-106.60(11)	P5	C43	C44	C45	176.0(4)
C13	P3	Pd2	S3	97.60(12)	P5	C43	C48	C47	-176.3(3)
C13	P3	Pd4	P2	99.79(11)	P5	C49	C50	C51	-175.8(3)
C13	P3	Pd4	P6	-80.04(11)	P5	C49	C54	C53	176.2(3)
C13	P3	Pd4	Pd1	110.03(11)	P5	Pd3	S1	P1	175.79(4)
C13	P3	Pd4	S2	109.48(12)	P6	C55	C56	C57	178.3(5)
C13	P3	S3	Pd2	-108.03(11)	P6	C55	C60	C59	-178.2(6)
C14	C13	C18	C17	-1.1(5)	P6	C61	C62	C63	-178.1(6)
C14	C13	P3	Pd1	37.9(3)	P6	C61	C66	C65	177.4(4)
C14	C13	P3	Pd2	108.3(3)	P6	C67	C68	C69	-178.8(3)
C14	C13	P3	Pd4	-41.8(3)	P6	C67	C72	C71	177.5(3)
C14	C13	P3	S3	171.5(2)	P6	Pd4	S2	P2	176.45(4)
C14	C15	C16	C17	-1.2(6)	Pd1	P1	Pd2	P3	-10.85(3)
C15	C16	C17	C18	0.8(7)	Pd1	P1	Pd2	P4	166.82(3)
C16	C17	C18	C13	0.3(6)	Pd1	P1	Pd2	S3	5.80(7)
C18	C13	C14	C15	0.7(5)	Pd1	P1	Pd3	P2	13.41(3)
C18	C13	P3	Pd1	-145.9(3)	Pd1	P1	Pd3	P5	-165.46(4)
C18	C13	P3	Pd2	-75.6(3)	Pd1	P1	Pd3	S1	-158.25(5)
C18	C13	P3	Pd4	134.3(3)	Pd1	P1	S1	Pd3	21.20(4)
C18	C13	P3	S3	-12.3(3)	Pd1	P2	Pd3	P1	-12.40(3)
C19	C20	C21	C22	0.8(7)	Pd	P2	Pd	P5	166.89(3)

					1		3		
C19	P4	Pd2	P1	161.50(14)	Pd1	P2	Pd3	S1	-1.70(7)
C19	P4	Pd2	P3	-23.27(16)	Pd1	P2	Pd4	P3	10.78(3)
C19	P4	Pd2	Pd1	-171.28(13)	Pd1	P2	Pd4	P6	-169.58(6)
C19	P4	Pd2	S3	-29.19(14)	Pd1	P2	Pd4	S2	-162.35(4)
C20	C19	C24	C23	0.5(6)	Pd1	P2	S2	Pd4	18.56(5)
C20	C19	P4	C25	-173.3(3)	Pd1	P3	Pd2	P1	11.49(3)
C20	C19	P4	C31	-63.6(3)	Pd1	P3	Pd2	P4	-163.78(6)
C20	C19	P4	Pd2	58.0(3)	Pd1	P3	Pd2	S3	-155.80(5)
C20	C21	C22	C23	0.6(8)	Pd1	P3	Pd4	P2	-10.25(3)
C21	C22	C23	C24	-1.4(8)	Pd1	P3	Pd4	P6	169.93(3)
C22	C23	C24	C19	0.9(7)	Pd1	P3	Pd4	S2	-0.56(7)
C24	C19	C20	C21	-1.3(6)	Pd1	P3	S3	Pd2	24.28(5)
C24	C19	P4	C25	10.8(4)	Pd1	Pd2	S3	P3	-18.33(4)
C24	C19	P4	C31	120.5(3)	Pd1	Pd3	S1	P1	-16.28(4)
C24	C19	P4	Pd2	-117.9(3)	Pd1	Pd4	S2	P2	-13.57(3)
C25	C26	C27	C28	1.3(7)	Pd2	P1	Pd1	P2	-157.91(3)
C25	P4	Pd2	P1	39.89(14)	Pd2	P1	Pd1	P3	14.71(4)
C25	P4	Pd2	P3	-144.88(14)	Pd2	P1	Pd1	Pd3	-142.54(3)
C25	P4	Pd2	Pd1	67.11(16)	Pd2	P1	Pd1	Pd4	-50.23(8)
C25	P4	Pd2	S3	-150.81(14)	Pd2	P1	Pd3	P2	55.58(5)
C26	C25	C30	C29	1.6(9)	Pd	P1	Pd	P5	-123.28(5)

					2		3		
C26	C25	P4	C19	-84.1(3)	Pd2	P1	Pd3	Pd1	42.17(3)
C26	C25	P4	C31	168.3(3)	Pd2	P1	Pd3	S1	-116.08(6)
C26	C25	P4	Pd2	44.0(3)	Pd2	P1	S1	Pd3	106.12(5)
C26	C27	C28	C29	-2.6(10)	Pd2	P3	Pd1	P1	-12.98(4)
C27	C28	C29	C30	3.5(13)	Pd2	P3	Pd1	P2	159.89(3)
C28	C29	C30	C25	-3.0(12)	Pd2	P3	Pd1	Pd3	95.15(6)
C30	C25	C26	C27	-0.8(7)	Pd2	P3	Pd1	Pd4	146.53(3)
C30	C25	P4	C19	91.8(5)	Pd2	P3	Pd4	P2	-46.86(4)
C30	C25	P4	C31	-15.8(5)	Pd2	P3	Pd4	P6	133.31(4)
C30	C25	P4	Pd2	-140.1(4)	Pd2	P3	Pd4	Pd1	-36.62(3)
C31	C32	C33	C34	-0.8(6)	Pd2	P3	Pd4	S2	-37.17(8)
C31	P4	Pd2	P1	-81.49(12)	Pd2	Pd1	Pd3	P1	-32.58(3)
C31	P4	Pd2	P3	93.74(13)	Pd2	Pd1	Pd3	P2	163.52(3)
C31	P4	Pd2	Pd1	-54.27(14)	Pd2	Pd1	Pd3	P5	117.54(8)
C31	P4	Pd2	S3	87.82(12)	Pd2	Pd1	Pd3	S1	-17.42(3)
C32	C31	C36	C35	-1.0(6)	Pd2	Pd1	Pd4	P2	-159.52(3)
C32	C31	P4	C19	-33.1(3)	Pd2	Pd1	Pd4	P3	33.43(3)
C32	C31	P4	C25	74.6(3)	Pd2	Pd1	Pd4	P6	7.82(7)
C32	C31	P4	Pd2	-157.8(3)	Pd2	Pd1	Pd4	S2	-146.86(2)
C32	C33	C34	C35	0.6(7)	Pd3	P1	Pd1	P2	-15.38(4)
C33	C34	C35	C36	-0.6(6)	Pd	P1	Pd	P3	157.25(3)

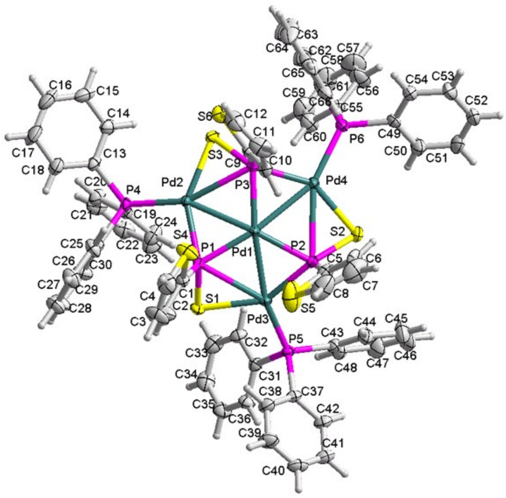
					3		1		
C34	C35	C36	C31	0.8(6)	Pd3	P1	Pd1	Pd2	142.54(3)
C36	C31	C32	C33	1.0(6)	Pd3	P1	Pd1	Pd4	92.30(7)
C36	C31	P4	C19	145.2(3)	Pd3	P1	Pd2	P3	-49.54(4)
C36	C31	P4	C25	-107.1(3)	Pd3	P1	Pd2	P4	128.14(4)
C36	C31	P4	Pd2	20.6(3)	Pd3	P1	Pd2	Pd1	-38.69(2)
C37	C38	C39	C40	-0.2(6)	Pd3	P1	Pd2	S3	-32.88(8)
C37	P5	Pd3	P1	32.35(14)	Pd3	P2	Pd1	P1	17.68(4)
C37	P5	Pd3	P2	-146.45(13)	Pd3	P2	Pd1	P3	-155.07(3)
C37	P5	Pd3	Pd1	-106.90(14)	Pd3	P2	Pd1	Pd2	-54.02(8)
C37	P5	Pd3	S1	27.19(13)	Pd3	P2	Pd1	Pd4	-143.21(3)
C38	C37	C42	C41	-0.9(7)	Pd3	P2	Pd4	P3	52.77(5)
C38	C37	P5	C43	165.2(3)	Pd3	P2	Pd4	P6	-127.59(6)
C38	C37	P5	C49	-89.5(3)	Pd3	P2	Pd4	Pd1	41.99(3)
C38	C37	P5	Pd3	40.9(3)	Pd3	P2	Pd4	S2	-120.36(6)
C38	C39	C40	C41	1.0(7)	Pd3	P2	S2	Pd4	108.48(5)
C39	C40	C41	C42	-1.7(9)	Pd3	Pd1	Pd2	P1	38.15(3)
C40	C41	C42	C37	1.7(9)	Pd3	Pd1	Pd2	P3	-155.69(3)
C42	C37	C38	C39	0.1(6)	Pd3	Pd1	Pd2	P4	5.15(7)
C42	C37	P5	C43	-14.8(4)	Pd3	Pd1	Pd2	S3	-138.67(3)
C42	C37	P5	C49	90.6(4)	Pd3	Pd1	Pd4	P2	-31.44(2)
C42	C37	P5	Pd	-139.1(3)	Pd	Pd	Pd	P3	161.51(3)

		3			3	1	4		
C43	C44	C45	C46	1.0(8)	Pd3	Pd1	Pd4	P6	135.90(7)
C43	P5	Pd3	P1	-85.33(13)	Pd3	Pd1	Pd4	S2	-18.78(3)
C43	P5	Pd3	P2	95.87(13)	Pd4	P2	Pd1	P1	160.89(3)
C43	P5	Pd3	Pd1	135.43(13)	Pd4	P2	Pd1	P3	-11.86(3)
C43	P5	Pd3	S1	-90.49(12)	Pd4	P2	Pd1	Pd2	89.19(7)
C44	C43	C48	C47	0.9(6)	Pd4	P2	Pd1	Pd3	143.21(3)
C44	C43	P5	C37	-92.1(3)	Pd4	P2	Pd3	P1	-52.04(5)
C44	C43	P5	C49	160.5(3)	Pd4	P2	Pd3	P5	127.25(4)
C44	C43	P5	Pd3	31.4(3)	Pd4	P2	Pd3	Pd1	-39.64(3)
C44	C45	C46	C47	-0.3(8)	Pd4	P2	Pd3	S1	-41.34(8)
C45	C46	C47	C48	0.0(7)	Pd4	P3	Pd1	P1	-159.51(3)
C46	C47	C48	C43	-0.3(6)	Pd4	P3	Pd1	P2	13.36(4)
C48	C43	C44	C45	-1.3(6)	Pd4	P3	Pd1	Pd2	-146.53(3)
C48	C43	P5	C37	85.0(3)	Pd4	P3	Pd1	Pd3	-51.38(7)
C48	C43	P5	C49	-22.4(3)	Pd4	P3	Pd2	P1	50.98(5)
C48	C43	P5	Pd3	-151.5(3)	Pd4	P3	Pd2	P4	-124.29(6)
C49	C50	C51	C52	-0.9(7)	Pd4	P3	Pd2	Pd1	39.49(3)
C49	P5	Pd3	P1	154.83(13)	Pd4	P3	Pd2	S3	-116.31(6)
C49	P5	Pd3	P2	-23.96(14)	Pd4	P3	S3	Pd2	111.62(5)
C49	P5	Pd3	Pd1	15.59(18)	Pd4	Pd1	Pd2	P1	164.88(3)
C49	P5	Pd	S1	149.68(14)	Pd	Pd	Pd	P3	-28.96(2)

		3			4	1	2		
C50	C49	C54	C53	-1.1(5)	Pd4	Pd1	Pd2	P4	131.89(6)
C50	C49	P5	C37	-4.4(3)	Pd4	Pd1	Pd2	S3	-11.94(3)
C50	C49	P5	C43	102.1(3)	Pd4	Pd1	Pd3	P1	-160.51(3)
C50	C49	P5	Pd3	-131.5(3)	Pd4	Pd1	Pd3	P2	35.59(3)
C50	C51	C52	C53	0.1(8)	Pd4	Pd1	Pd3	P5	-10.39(9)
C51	C52	C53	C54	0.2(8)	Pd4	Pd1	Pd3	S1	-145.35(3)
C52	C53	C54	C49	0.3(7)	S1	P1	Pd1	P2	-35.45(6)
C54	C49	C50	C51	1.4(6)	S1	P1	Pd1	P3	137.18(5)
C54	C49	P5	C37	178.4(3)	S1	P1	Pd1	Pd2	122.46(6)
C54	C49	P5	C43	-75.1(3)	S1	P1	Pd1	Pd3	-20.07(4)
C54	C49	P5	Pd3	51.4(3)	S1	P1	Pd1	Pd4	72.23(9)
C55	C56	C57	C58	0.9(12)	S1	P1	Pd2	P3	-119.05(6)
C55	P6	Pd4	P2	67.19(17)	S1	P1	Pd2	P4	58.62(6)
C55	P6	Pd4	P3	-113.17(16)	S1	P1	Pd2	Pd1	-108.20(6)
C55	P6	Pd4	Pd1	-91.94(17)	S1	P1	Pd2	S3	-102.40(7)
C55	P6	Pd4	S2	61.78(16)	S1	P1	Pd3	P2	171.66(4)
C56	C55	C60	C59	-1.8(10)	S1	P1	Pd3	P5	-7.20(7)
C56	C55	P6	C61	162.0(4)	S1	P1	Pd3	Pd1	158.25(5)
C56	C55	P6	C67	-91.5(4)	S2	P2	Pd1	P1	143.16(5)
C56	C55	P6	Pd4	36.8(4)	S2	P2	Pd1	P3	-29.59(7)
C56	C57	C58	C59	-3.7(15)	S2	P2	Pd	Pd	71.46(9)

							1	2	
C57	C58	C59	C60	3.7(17)	S2	P2	Pd1	Pd3	125.48(6)
C58	C59	C60	C55	-0.8(14)	S2	P2	Pd1	Pd4	-17.73(4)
C60	C55	C56	C57	1.8(9)	S2	P2	Pd3	P1	-127.18(5)
C60	C55	P6	C61	-21.6(5)	S2	P2	Pd3	P5	52.11(6)
C60	C55	P6	C67	84.9(5)	S2	P2	Pd3	Pd1	-114.78(6)
C60	C55	P6	Pd4	-146.8(4)	S2	P2	Pd3	S1	-116.49(7)
C61	C62	C63	C64	-0.1(12)	S2	P2	Pd4	P3	173.13(4)
C61	P6	Pd4	P2	-52.29(17)	S2	P2	Pd4	P6	-7.23(8)
C61	P6	Pd4	P3	127.35(15)	S2	P2	Pd4	Pd1	162.35(4)
C61	P6	Pd4	Pd1	148.59(15)	S3	P3	Pd1	P1	-36.17(7)
C61	P6	Pd4	S2	-57.69(15)	S3	P3	Pd1	P2	136.71(5)
C62	C61	C66	C65	-0.7(8)	S3	P3	Pd1	Pd2	-23.19(5)
C62	C61	P6	C55	-95.9(5)	S3	P3	Pd1	Pd3	71.97(8)
C62	C61	P6	C67	156.6(4)	S3	P3	Pd1	Pd4	123.34(6)
C62	C61	P6	Pd4	27.4(5)	S3	P3	Pd2	P1	167.29(4)
C62	C63	C64	C65	0.6(12)	S3	P3	Pd2	P4	-7.98(8)
C63	C64	C65	C66	-1.1(11)	S3	P3	Pd2	Pd1	155.80(5)
C64	C65	C66	C61	1.2(9)	S3	P3	Pd4	P2	-121.16(5)
C66	C61	C62	C63	0.2(9)	S3	P3	Pd4	P6	59.02(6)
C66	C61	P6	C55	86.0(4)	S3	P3	Pd4	Pd1	-110.91(6)
C66	C61	P6	C67	-21.5(5)	S3	P3	Pd	S2	-111.47(7)

			4	
C66	C61	P6	Pd4	-150.7(4)



2c

Table 1 Crystal data and structure refinement for 2c.

Empirical formula	$C_{66}H_{54}P_6Pd_4S_6$
Formula weight	1650.87
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	15.6070(3)
b/Å	27.8868(3)
c/Å	17.6155(3)
α/°	90
β/°	112.931(2)
γ/°	90
Volume/Å^3	7060.9(2)
Z	4
ρ_{calc}g/cm^3	1.553
μ/mm^{-1}	1.353
F(000)	3280.0
Crystal size/mm^3	0.21 × 0.17 × 0.16
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.818 to 52.742
Index ranges	-19 ≤ h ≤ 19, -34 ≤ k ≤ 34, -22 ≤ l ≤ 20

Reflections collected	37057
Independent reflections	14396 [R_{int} = 0.0324, R_{sigma} = 0.0425]
Data/restraints/parameters	14396/35/760
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0388, wR_2 = 0.0935
Final R indexes [all data]	R_1 = 0.0522, wR_2 = 0.1000
Largest diff. peak/hole / e Å^{-3}	1.28/-0.85

Table 2 Bond Lengths for 2c.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.390(10)	C35	C36	1.391(6)
C1	C2A	1.394(17)	C37	C38	1.379(6)
C1	P1	1.793(4)	C37	C42	1.393(5)
C1	S4	1.702(4)	C37	P5	1.833(4)
C1	S4A	1.636(10)	C38	C39	1.386(6)
C2	C3	1.365(10)	C39	C40	1.381(7)
C2A	C4	1.420(17)	C40	C41	1.365(7)
C3	C4	1.315(7)	C41	C42	1.386(6)
C3	S4A	1.669(10)	C43	C44	1.393(6)
C4	S4	1.653(6)	C43	C48	1.385(6)
C5	C6	1.418(10)	C43	P5	1.816(4)
C5	C6A	1.437(11)	C44	C45	1.389(7)
C5	P2	1.815(4)	C45	C46	1.372(9)
C5	S5	1.715(7)	C46	C47	1.368(9)
C5	S5A	1.724(7)	C47	C48	1.397(7)
C6	C7	1.309(9)	C49	C50	1.387(6)
C6A	C8	1.324(10)	C49	C54	1.376(6)
C7	C8	1.276(9)	C49	P6	1.837(4)
C7	S5A	1.742(9)	C50	C51	1.380(6)
C8	S5	1.789(9)	C51	C52	1.350(7)
C9	C10	1.459(18)	C52	C53	1.372(7)
C9	C10A	1.424(11)	C53	C54	1.397(6)
C9	P3	1.806(4)	C55	C56	1.378(6)
C9	S6	1.702(7)	C55	C60	1.374(6)
C9	S6A	1.740(5)	C55	P6	1.828(5)
C10	C11	1.390(15)	C56	C57	1.401(8)
C10A	C12	1.326(11)	C57	C58	1.351(10)
C11	C12	1.339(8)	C58	C59	1.348(9)
C11	S6A	1.690(7)	C59	C60	1.398(7)

C12	S6	1.689(7)	C61	C62	1.380(8)
C13	C14	1.387(6)	C61	C66	1.379(7)
C13	C18	1.394(6)	C61	P6	1.828(5)
C13	P4	1.833(4)	C62	C63	1.419(9)
C14	C15	1.393(6)	C63	C64	1.348(10)
C15	C16	1.371(8)	C64	C65	1.367(10)
C16	C17	1.355(9)	C65	C66	1.393(7)
C17	C18	1.370(7)	P1	Pd1	2.2622(9)
C19	C20	1.392(5)	P1	Pd2	2.2752(10)
C19	C24	1.376(6)	P1	Pd3	2.7875(10)
C19	P4	1.829(4)	P1	S1	2.0141(14)
C20	C21	1.385(6)	P2	Pd1	2.2804(9)
C21	C22	1.357(7)	P2	Pd3	2.2927(10)
C22	C23	1.366(7)	P2	Pd4	2.7467(10)
C23	C24	1.375(6)	P2	S2	2.0220(14)
C25	C26	1.382(6)	P3	Pd1	2.2707(9)
C25	C30	1.383(6)	P3	Pd2	2.7322(9)
C25	P4	1.827(4)	P3	Pd4	2.2830(9)
C26	C27	1.393(6)	P3	S3	2.0213(13)
C27	C28	1.358(7)	P4	Pd2	2.2911(9)
C28	C29	1.361(7)	P5	Pd3	2.3006(10)
C29	C30	1.391(6)	P6	Pd4	2.2928(10)
C31	C32	1.389(6)	Pd1	Pd2	2.6668(4)
C31	C36	1.386(5)	Pd1	Pd3	2.6536(4)
C31	P5	1.832(4)	Pd1	Pd4	2.6669(4)
C32	C33	1.375(6)	Pd2	S3	2.4211(10)
C33	C34	1.363(7)	Pd3	S1	2.4100(10)
C34	C35	1.377(7)	Pd4	S2	2.4152(11)

Table 3 Bond Angles for 2c.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	P1	133.0(5)	C63	C64	C65	122.9(7)
C2	C1	S4	107.0(5)	C64	C65	C66	118.2(7)
C2A	C1	P1	132.1(9)	C61	C66	C65	121.0(6)
C2A	C1	S4A	108.3(10)	C1	P1	Pd1	112.12(13)
S4	C1	P1	119.9(2)	C1	P1	Pd2	115.38(13)
S4A	C1	P1	119.6(4)	C1	P1	Pd3	112.89(13)
C3	C2	C1	115.4(8)	C1	P1	S1	107.78(14)
C1	C2A	C4	118.6(16)	Pd1	P1	Pd2	71.99(3)
C4	C3	C2	110.2(6)	Pd1	P1	Pd3	62.38(2)
C4	C3	S4A	121.2(5)	Pd2	P1	Pd3	122.64(4)
C3	C4	C2A	100.2(10)	S1	P1	Pd1	116.72(5)
C3	C4	S4	114.8(4)	S1	P1	Pd2	128.10(6)
C6	C5	P2	135.7(5)	S1	P1	Pd3	57.59(4)
C6	C5	S5	108.3(5)	C5	P2	Pd1	105.17(14)
C6A	C5	P2	133.1(5)	C5	P2	Pd3	115.17(16)
C6A	C5	S5A	107.5(5)	C5	P2	Pd4	106.64(15)
S5	C5	P2	114.8(3)	C5	P2	S2	106.82(16)
S5A	C5	P2	117.8(3)	Pd1	P2	Pd3	70.94(3)
C7	C6	C5	119.4(9)	Pd1	P2	Pd4	63.28(2)
C8	C6A	C5	118.6(9)	Pd3	P2	Pd4	124.05(4)
C8	C7	C6	105.9(8)	S2	P2	Pd1	119.11(5)
C8	C7	S5A	122.0(6)	S2	P2	Pd3	132.31(6)
C7	C8	C6A	105.2(8)	S2	P2	Pd4	58.53(4)
C7	C8	S5	119.5(6)	C9	P3	Pd1	112.03(13)
C10	C9	P3	129.6(6)	C9	P3	Pd2	110.78(12)
C10	C9	S6	109.5(7)	C9	P3	Pd4	113.45(13)
C10A	C9	P3	137.0(5)	C9	P3	S3	107.49(14)
C10A	C9	S6A	106.9(5)	Pd1	P3	Pd2	63.64(2)
S6	C9	P3	120.8(3)	Pd1	P3	Pd4	71.70(3)
S6A	C9	P3	116.1(2)	Pd4	P3	Pd2	125.78(4)
C11	C10	C9	114.8(12)	S3	P3	Pd1	118.39(5)
C12	C10A	C9	118.2(9)	S3	P3	Pd2	59.00(4)

C12	C11	C10	104.6(9)	S3	P3	Pd4	129.34(6)
C12	C11	S6A	118.4(4)	C13	P4	Pd2	118.21(13)
C10A	C12	C11	107.3(7)	C19	P4	C13	103.69(18)
C11	C12	S6	121.4(5)	C19	P4	Pd2	113.33(13)
C14	C13	C18	118.1(4)	C25	P4	C13	103.32(19)
C14	C13	P4	118.2(3)	C25	P4	C19	102.70(18)
C18	C13	P4	123.7(4)	C25	P4	Pd2	113.83(12)
C13	C14	C15	120.7(5)	C31	P5	C37	103.13(18)
C16	C15	C14	118.6(6)	C31	P5	Pd3	112.15(12)
C17	C16	C15	121.9(5)	C37	P5	Pd3	115.58(13)
C16	C17	C18	119.5(6)	C43	P5	C31	103.62(18)
C17	C18	C13	121.2(6)	C43	P5	C37	103.03(19)
C20	C19	P4	122.4(3)	C43	P5	Pd3	117.61(13)
C24	C19	C20	118.7(4)	C49	P6	Pd4	118.61(13)
C24	C19	P4	118.8(3)	C55	P6	C49	102.37(19)
C21	C20	C19	119.3(4)	C55	P6	Pd4	114.50(15)
C22	C21	C20	121.2(4)	C61	P6	C49	103.04(19)
C21	C22	C23	119.6(4)	C61	P6	C55	104.5(2)
C22	C23	C24	120.4(5)	C61	P6	Pd4	112.14(15)
C23	C24	C19	120.8(4)	P1	Pd1	P2	121.11(4)
C26	C25	C30	117.9(4)	P1	Pd1	P3	118.84(3)
C26	C25	P4	123.4(3)	P1	Pd1	Pd2	54.23(3)
C30	C25	P4	118.6(3)	P1	Pd1	Pd3	68.56(3)
C25	C26	C27	120.6(4)	P1	Pd1	Pd4	164.57(3)
C28	C27	C26	120.7(5)	P2	Pd1	Pd2	162.80(3)
C27	C28	C29	119.6(5)	P2	Pd1	Pd3	54.75(3)
C28	C29	C30	120.5(5)	P2	Pd1	Pd4	66.92(3)
C25	C30	C29	120.7(4)	P3	Pd1	P2	120.00(3)
C32	C31	P5	119.0(3)	P3	Pd1	Pd2	66.64(2)
C36	C31	C32	118.3(4)	P3	Pd1	Pd3	161.64(3)
C36	C31	P5	122.7(3)	P3	Pd1	Pd4	54.36(2)
C33	C32	C31	121.3(4)	Pd2	Pd1	Pd4	113.831(13)
C34	C33	C32	120.1(5)	Pd3	Pd1	Pd2	113.463(13)
C33	C34	C35	119.9(5)	Pd3	Pd1	Pd4	113.742(13)
C34	C35	C36	120.4(5)	P1	Pd2	P3	102.02(3)
C31	C36	C35	119.9(4)	P1	Pd2	P4	101.53(4)
C38	C37	C42	118.7(4)	P1	Pd2	Pd1	53.78(2)
C38	C37	P5	118.5(3)	P1	Pd2	S3	146.59(3)
C42	C37	P5	122.6(3)	P4	Pd2	P3	156.45(3)
C37	C38	C39	120.4(4)	P4	Pd2	Pd1	152.60(3)

C40	C39	C38	120.0(5)	P4	Pd2	S3	110.98(4)
C41	C40	C39	120.4(4)	Pd1	Pd2	P3	49.72(2)
C40	C41	C42	119.7(5)	S3	Pd2	P3	45.69(3)
C41	C42	C37	120.8(4)	S3	Pd2	Pd1	92.81(3)
C44	C43	P5	118.1(3)	P2	Pd3	P1	101.83(3)
C48	C43	C44	118.8(4)	P2	Pd3	P5	114.22(4)
C48	C43	P5	123.1(3)	P2	Pd3	Pd1	54.31(2)
C45	C44	C43	121.2(5)	P2	Pd3	S1	146.14(4)
C46	C45	C44	119.1(6)	P5	Pd3	P1	143.92(3)
C47	C46	C45	120.6(6)	P5	Pd3	Pd1	163.23(3)
C46	C47	C48	120.7(6)	P5	Pd3	S1	99.15(4)
C43	C48	C47	119.5(5)	Pd1	Pd3	P1	49.06(2)
C50	C49	P6	118.3(3)	S1	Pd3	P1	44.87(3)
C54	C49	C50	117.6(4)	S1	Pd3	Pd1	91.89(3)
C54	C49	P6	124.0(3)	P3	Pd4	P2	102.80(3)
C51	C50	C49	120.4(5)	P3	Pd4	P6	102.66(4)
C52	C51	C50	121.6(5)	P3	Pd4	Pd1	53.94(2)
C51	C52	C53	119.4(5)	P3	Pd4	S2	147.63(4)
C52	C53	C54	119.6(5)	P6	Pd4	P2	154.30(3)
C49	C54	C53	121.3(5)	P6	Pd4	Pd1	155.84(3)
C56	C55	P6	121.9(4)	P6	Pd4	S2	109.47(4)
C60	C55	C56	119.0(5)	Pd1	Pd4	P2	49.80(2)
C60	C55	P6	119.0(4)	S2	Pd4	P2	45.56(3)
C55	C56	C57	119.3(6)	S2	Pd4	Pd1	93.69(3)
C58	C57	C56	120.7(7)	P1	S1	Pd3	77.54(4)
C59	C58	C57	120.7(6)	P2	S2	Pd4	75.91(4)
C58	C59	C60	119.6(6)	P3	S3	Pd2	75.31(4)
C55	C60	C59	120.7(6)	C4	S4	C1	92.3(3)
C62	C61	C66	119.5(5)	C1	S4A	C3	89.6(5)
C62	C61	P6	122.0(4)	C5	S5	C8	85.3(3)
C66	C61	P6	118.4(4)	C5	S5A	C7	85.7(4)
C61	C62	C63	119.6(7)	C12	S6	C9	88.2(3)
C64	C63	C62	118.8(7)	C11	S6A	C9	88.9(3)

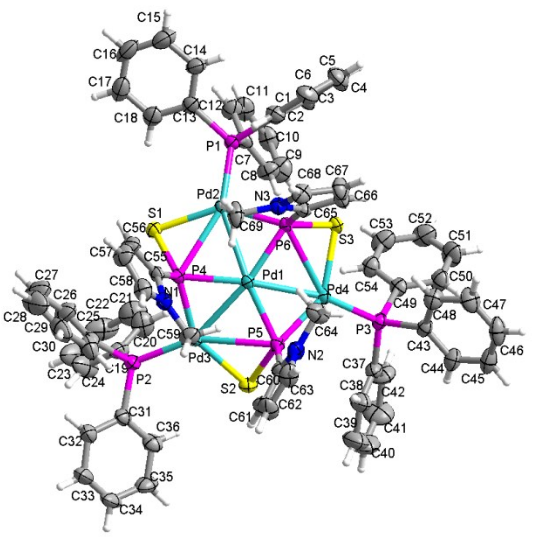
Table 4 Torsion Angles for 2c.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	5.9(12)	C42	C37	P5	C31	91.5(4)
C1	C2	C3	S4A	-129(3)	C42	C37	P5	C43	-16.1(4)
C1	C2A	C4	C3	-9.5(18)	C42	C37	P5	Pd3	-145.7(3)
C1	C2A	C4	S4	147(5)	C43	C44	C45	C46	2.2(10)
C2	C1	C2A	C4	12.0(17)	C44	C43	C48	C47	0.4(7)
C2	C1	P1	Pd1	-143.7(7)	C44	C43	P5	C31	-178.7(4)
C2	C1	P1	Pd2	136.5(7)	C44	C43	P5	C37	-71.5(4)
C2	C1	P1	Pd3	-75.5(7)	C44	C43	P5	Pd3	56.9(4)
C2	C1	P1	S1	-13.9(8)	C44	C45	C46	C47	-0.7(12)
C2	C1	S4	C4	1.0(6)	C45	C46	C47	C48	-1.0(12)
C2	C1	S4A	C3	-33(2)	C46	C47	C48	C43	1.1(10)
C2	C3	C4	C2A	1.9(12)	C48	C43	C44	C45	-2.0(8)
C2	C3	C4	S4	-5.0(9)	C48	C43	P5	C31	0.6(4)
C2	C3	S4A	C1	37(2)	C48	C43	P5	C37	107.8(4)
C2A	C1	C2	C3	-10.2(13)	C48	C43	P5	Pd3	-123.8(4)
C2A	C1	P1	Pd1	47.9(13)	C49	C50	C51	C52	1.2(8)

C2A	C1	P1	Pd2	-31.9(13)	C50	C49	C54	C53	-0.8(7)
C2A	C1	P1	Pd3	116.1(13)	C50	C49	P6	C55	-73.7(4)
C2A	C1	P1	S1	177.7(13)	C50	C49	P6	C61	178.0(4)
C2A	C1	S4	C4	27(4)	C50	C49	P6	Pd4	53.4(4)
C2A	C1	S4A	C3	6.5(10)	C50	C51	C52	C53	0.0(9)
C2A	C4	S4	C1	-23(3)	C51	C52	C53	C54	-1.5(8)
C3	C4	S4	C1	2.4(5)	C52	C53	C54	C49	1.9(8)
C4	C3	S4A	C1	-14.5(8)	C54	C49	C50	C51	-0.8(7)
C5	C6	C7	C8	-14.1(13)	C54	C49	P6	C55	105.0(4)
C5	C6	C7	S5A	147(3)	C54	C49	P6	C61	-3.4(4)
C5	C6A	C8	C7	10.4(13)	C54	C49	P6	Pd4	-127.9(3)
C5	C6A	C8	S5	-140(3)	C55	C56	C57	C58	0.2(12)
C6	C5	C6A	C8	-15.8(10)	C56	C55	C60	C59	0.2(9)
C6	C5	P2	Pd1	-111.6(7)	C56	C55	P6	C49	-35.0(5)
C6	C5	P2	Pd3	172.7(7)	C56	C55	P6	C61	72.2(5)
C6	C5	P2	Pd4	-45.5(8)	C56	C55	P6	Pd4	-164.7(4)
C6	C5	P2	S2	15.9(8)	C56	C57	C58	C59	-0.2(13)
C6	C5	S5	C8	-3.2(6)	C57	C58	C59	C60	0.1(13)
C6	C5	S5A	C7	17.9(16)	C58	C59	C60	C55	-0.1(10)
C6	C7	C8	C6A	1.9(12)	C60	C55	C56	C57	-0.2(9)
C6	C7	C8	S5	11.2(12)	C60	C55	P6	C49	147.4(4)
C6	C7	S5A	C5	-23(2)	C60	C55	P6	C61	-105.5(4)
C6A	C5	C6	C7	17.3(10)	C60	C55	P6	Pd4	17.7(5)
C6A	C5	P2	Pd1	40.6(8)	C61	C62	C63	C64	0.0(11)
C6A	C5	P2	Pd3	-35.2(8)	C62	C61	C66	C65	-0.9(7)
C6A	C5	P2	Pd4	106.7(7)	C62	C61	P6	C49	115.2(4)
C6A	C5	P2	S2	168.0(7)	C62	C61	P6	C55	8.5(5)
C6A	C5	S5	C8	-20.1(14)	C62	C61	P6	Pd4	-116.1(4)
C6A	C5	S5A	C7	6.7(7)	C62	C63	C64	C65	-0.2(13)
C6A	C8	S5	C5	28(2)	C63	C64	C65	C66	-0.2(11)
C7	C8	S5	C5	-4.8(8)	C64	C65	C66	C61	0.7(8)
C8	C7	S5A	C5	-1.7(9)	C66	C61	C62	C63	0.5(9)
C9	C10	C11	C12	13.0(11)	C66	C61	P6	C49	-67.6(4)
C9	C10	C11	S6A	-137(3)	C66	C61	P6	C55	-174.3(3)
C9	C10A	C12	C11	-6.6(10)	C66	C61	P6	Pd4	61.0(4)
C9	C10A	C12	S6	153(3)	P1	C1	C2	C3	178.4(5)
C10	C9	C10A	C12	12.7(9)	P1	C1	C2A	C4	-176.5(8)
C10	C9	P3	Pd1	34.8(8)	P1	C1	S4	C4	178.9(3)
C10	C9	P3	Pd2	103.8(8)	P1	C1	S4A	C3	-175.9(3)
C10	C9	P3	Pd4	-44.0(8)	P2	C5	C6	C7	177.3(6)

C10	C9	P3	S3	166.5(8)	P2	C5	C6A	C8	-176.7(6)
C10	C9	S6	C12	4.4(7)	P2	C5	S5	C8	-172.6(3)
C10	C9	S6A	C11	-30(2)	P2	C5	S5A	C7	174.2(4)
C10	C11	C12	C10A	-3.9(9)	P3	C9	C10	C11	172.9(5)
C10	C11	C12	S6	-10.1(9)	P3	C9	C10A	C12	-176.0(4)
C10	C11	S6A	C9	32(3)	P3	C9	S6	C12	-179.4(3)
C10A	C9	C10	C11	-14.9(10)	P3	C9	S6A	C11	179.4(3)
C10A	C9	P3	Pd1	-133.8(7)	P4	C13	C14	C15	178.8(3)
C10A	C9	P3	Pd2	-64.8(7)	P4	C13	C18	C17	179.9(4)
C10A	C9	P3	Pd4	147.3(7)	P4	C19	C20	C21	-175.4(4)
C10A	C9	P3	S3	-2.1(7)	P4	C19	C24	C23	175.6(4)
C10A	C9	S6	C12	16.5(17)	P4	C25	C26	C27	-179.8(4)
C10A	C9	S6A	C11	-1.4(5)	P4	C25	C30	C29	179.3(4)
C10A	C12	S6	C9	-20(2)	P5	C31	C32	C33	179.8(3)
C11	C12	S6	C9	3.5(6)	P5	C31	C36	C35	179.8(3)
C12	C11	S6A	C9	-2.3(5)	P5	C37	C38	C39	175.6(4)
C13	C14	C15	C16	1.4(7)	P5	C37	C42	C41	-176.1(3)
C14	C13	C18	C17	-1.9(8)	P5	C43	C44	C45	177.3(5)
C14	C13	P4	C19	-77.8(3)	P5	C43	C48	C47	-178.9(4)
C14	C13	P4	C25	175.3(3)	P6	C49	C50	C51	178.0(4)
C14	C13	P4	Pd2	48.6(4)	P6	C49	C54	C53	-179.4(4)
C14	C15	C16	C17	-2.0(9)	P6	C55	C56	C57	-177.9(5)
C15	C16	C17	C18	0.6(10)	P6	C55	C60	C59	177.9(5)
C16	C17	C18	C13	1.4(10)	P6	C61	C62	C63	177.6(5)
C18	C13	C14	C15	0.5(6)	P6	C61	C66	C65	-178.1(4)
C18	C13	P4	C19	100.4(4)	S4	C1	C2	C3	-4.1(10)
C18	C13	P4	C25	-6.5(4)	S4	C1	C2A	C4	-143(5)
C18	C13	P4	Pd2	-133.2(4)	S4	C1	P1	Pd1	39.1(3)
C19	C20	C21	C22	0.3(7)	S4	C1	P1	Pd2	-40.7(3)
C20	C19	C24	C23	-0.5(7)	S4	C1	P1	Pd3	107.3(2)
C20	C19	P4	C13	-18.3(4)	S4	C1	P1	S1	168.9(2)
C20	C19	P4	C25	89.0(4)	S4	C1	S4A	C3	15.9(7)
C20	C19	P4	Pd2	-147.7(3)	S4A	C1	C2	C3	133(3)
C20	C21	C22	C23	-1.3(8)	S4A	C1	C2A	C4	0.7(18)
C21	C22	C23	C24	1.5(8)	S4A	C1	P1	Pd1	-129.1(5)
C22	C23	C24	C19	-0.6(8)	S4A	C1	P1	Pd2	151.1(5)
C24	C19	C20	C21	0.6(7)	S4A	C1	P1	Pd3	-60.9(5)
C24	C19	P4	C13	165.7(4)	S4A	C1	P1	S1	0.7(5)
C24	C19	P4	C25	-86.9(4)	S4A	C1	S4	C4	-13.0(6)
C24	C19	P4	Pd2	36.3(4)	S4A	C3	C4	C2A	15.5(13)

C25	C26	C27	C28	-1.1(8)	S4A	C3	C4	S4	8.6(9)
C26	C25	C30	C29	-2.9(7)	S5	C5	C6	C7	11.2(11)
C26	C25	P4	C13	109.0(4)	S5	C5	C6A	C8	148(2)
C26	C25	P4	C19	1.3(4)	S5	C5	P2	Pd1	53.9(3)
C26	C25	P4	Pd2	-121.6(4)	S5	C5	P2	Pd3	-21.8(4)
C26	C27	C28	C29	0.0(9)	S5	C5	P2	Pd4	120.0(3)
C27	C28	C29	C30	-0.4(9)	S5	C5	P2	S2	-178.6(3)
C28	C29	C30	C25	1.9(8)	S5	C5	S5A	C7	-2.2(6)
C30	C25	C26	C27	2.5(7)	S5A	C5	C6	C7	-152(2)
C30	C25	P4	C13	-73.3(4)	S5A	C5	C6A	C8	-12.0(11)
C30	C25	P4	C19	179.1(3)	S5A	C5	P2	Pd1	-123.0(3)
C30	C25	P4	Pd2	56.1(4)	S5A	C5	P2	Pd3	161.3(3)
C31	C32	C33	C34	0.4(7)	S5A	C5	P2	Pd4	-56.9(4)
C32	C31	C36	C35	0.2(6)	S5A	C5	P2	S2	4.5(4)
C32	C31	P5	C37	167.0(3)	S5A	C5	S5	C8	3.9(6)
C32	C31	P5	C43	-85.9(3)	S5A	C7	C8	C6A	-4.5(12)
C32	C31	P5	Pd3	42.0(4)	S5A	C7	C8	S5	4.9(12)
C32	C33	C34	C35	0.0(8)	S6	C9	C10	C11	-11.4(12)
C33	C34	C35	C36	-0.4(8)	S6	C9	C10A	C12	-156(2)
C34	C35	C36	C31	0.2(7)	S6	C9	P3	Pd1	-140.6(3)
C36	C31	C32	C33	-0.5(6)	S6	C9	P3	Pd2	-71.6(3)
C36	C31	P5	C37	-12.6(4)	S6	C9	P3	Pd4	140.6(3)
C36	C31	P5	C43	94.5(4)	S6	C9	P3	S3	-8.9(3)
C36	C31	P5	Pd3	-137.6(3)	S6	C9	S6A	C11	5.2(4)
C37	C38	C39	C40	0.8(8)	S6A	C9	C10	C11	138(3)
C38	C37	C42	C41	-0.2(7)	S6A	C9	C10A	C12	5.1(9)
C38	C37	P5	C31	-84.4(4)	S6A	C9	P3	Pd1	45.0(3)
C38	C37	P5	C43	168.0(3)	S6A	C9	P3	Pd2	114.0(2)
C38	C37	P5	Pd3	38.3(4)	S6A	C9	P3	Pd4	-33.8(3)
C38	C39	C40	C41	-0.3(8)	S6A	C9	P3	S3	176.74(19)
C39	C40	C41	C42	-0.4(8)	S6A	C9	S6	C12	-5.4(4)
C40	C41	C42	C37	0.7(7)	S6A	C11	C12	C10A	5.4(8)
C42	C37	C38	C39	-0.6(7)	S6A	C11	C12	S6	-0.9(7)



2d

Table 1 Crystal data and structure refinement for 2d.

Empirical formula	$C_{139}H_{128}Cl_2N_6P_{12}Pd_8S_6$
Formula weight	3368.57
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	16.0071(6)
b/Å	27.7820(9)
c/Å	17.5250(6)
α/°	90
β/°	113.968(4)
γ/°	90
Volume/Å^3	7121.5(5)
Z	2
ρ_{calc}g/cm^3	1.571
μ/mm^{-1}	10.786
F(000)	3364.0
Crystal size/mm^3	0.15 × 0.1 × 0.08
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.78 to 134.156
Index ranges	-19 ≤ h ≤ 18, -33 ≤ k ≤ 32, -20 ≤ l ≤ 18
Reflections collected	36504
Independent reflections	12702 [R_{int} = 0.0484, R_{sigma} = 0.0545]
Data/restraints/parameters	12702/20/796
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0529, wR_2 = 0.1377
Final R indexes [all data]	R_1 = 0.0767, wR_2 = 0.1549
Largest diff. peak/hole / e Å^{-3}	1.37/-0.62

Table 2 Bond Lengths for 2d.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.381(11)	C46	C47	1.380(17)
C1	C6	1.385(11)	C47	C48	1.380(14)
C1	P1	1.829(8)	C49	C50	1.391(12)
C2	C3	1.378(13)	C49	C54	1.377(13)
C3	C4	1.377(15)	C49	P3	1.837(8)
C4	C5	1.361(15)	C50	C51	1.390(14)
C5	C6	1.397(14)	C51	C52	1.359(17)
C7	C8	1.382(12)	C52	C53	1.376(16)
C7	C12	1.389(12)	C53	C54	1.373(13)

C7	P1	1.823(8)	C55	C56	1.370(11)
C8	C9	1.402(13)	C55	N1	1.377(10)
C9	C10	1.354(15)	C55	P4	1.793(7)
C10	C11	1.358(15)	C56	C57	1.386(13)
C11	C12	1.382(13)	C57	C58	1.340(14)
C13	C14	1.372(13)	C58	N1	1.376(10)
C13	C18	1.388(13)	C59	N1	1.435(11)
C13	P1	1.829(9)	C60	C61	1.384(12)
C14	C15	1.382(15)	C60	N2	1.375(11)
C15	C16	1.33(2)	C60	P5	1.813(8)
C16	C17	1.359(19)	C61	C62	1.393(14)
C17	C18	1.377(14)	C62	C63	1.361(15)
C19	C20	1.361(15)	C63	N2	1.367(11)
C19	C24	1.373(14)	C64	N2	1.433(11)
C19	P2	1.827(9)	C65	C66	1.361(11)
C20	C21	1.377(16)	C65	N3	1.392(10)
C21	C22	1.32(2)	C65	P6	1.790(8)
C22	C23	1.37(2)	C66	C67	1.406(13)
C23	C24	1.404(18)	C67	C68	1.348(13)
C25	C26	1.361(15)	C68	N3	1.367(11)
C25	C30	1.370(14)	C69	N3	1.435(11)
C25	P2	1.821(9)	P1	Pd2	2.2896(19)
C26	C27	1.402(17)	P2	Pd3	2.287(2)
C27	C28	1.37(2)	P3	Pd4	2.2887(19)
C28	C29	1.35(2)	P4	Pd1	2.2885(18)
C29	C30	1.391(16)	P4	Pd2	2.7577(18)
C31	C32	1.375(13)	P4	Pd3	2.2696(19)
C31	C36	1.382(13)	P4	S1	2.024(3)
C31	P2	1.836(9)	P5	Pd1	2.2926(19)
C32	C33	1.398(14)	P5	Pd3	2.777(2)
C33	C34	1.315(17)	P5	Pd4	2.2858(19)
C34	C35	1.381(16)	P5	S2	2.019(3)
C35	C36	1.389(13)	P6	Pd1	2.2742(19)
C37	C38	1.364(15)	P6	Pd2	2.2705(19)
C37	C42	1.382(14)	P6	Pd4	2.8139(19)
C37	P3	1.822(9)	P6	S3	2.016(3)
C38	C39	1.405(17)	Pd1	Pd2	2.6672(7)
C39	C40	1.36(2)	Pd1	Pd3	2.6655(7)
C40	C41	1.34(2)	Pd1	Pd4	2.6499(7)
C41	C42	1.396(17)	Pd2	S1	2.414(2)

C43	C44	1.406(12)	Pd3	S2	2.410(2)
C43	C48	1.374(13)	Pd4	S3	2.407(2)
C43	P3	1.828(8)	C70	Cl1	1.681(18)
C44	C45	1.384(14)	C70	Cl2	1.640(18)
C45	C46	1.354(17)			

Table3 Bond Angles for 2d.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	C6	118.6(8)	C63	N2	C64	123.0(8)
C2	C1	P1	118.8(6)	C1	P1	Pd2	113.5(3)
C6	C1	P1	122.6(7)	C7	P1	C1	103.7(4)
C3	C2	C1	120.8(9)	C7	P1	C13	102.8(4)
C4	C3	C2	120.6(10)	C7	P1	Pd2	112.2(3)
C5	C4	C3	119.0(10)	C13	P1	C1	103.0(4)
C4	C5	C6	121.1(10)	C13	P1	Pd2	119.9(3)
C1	C6	C5	119.7(9)	C19	P2	C31	103.3(4)
C8	C7	C12	118.6(8)	C19	P2	Pd3	113.8(3)
C8	C7	P1	117.8(6)	C25	P2	C19	104.2(5)
C12	C7	P1	123.6(7)	C25	P2	C31	104.2(4)
C7	C8	C9	119.4(9)	C25	P2	Pd3	111.7(3)
C10	C9	C8	120.8(11)	C31	P2	Pd3	118.3(3)
C9	C10	C11	120.3(9)	C37	P3	C43	103.8(4)
C10	C11	C12	120.2(9)	C37	P3	C49	103.7(4)
C11	C12	C7	120.7(10)	C37	P3	Pd4	117.5(3)
C14	C13	C18	118.4(9)	C43	P3	C49	101.3(4)
C14	C13	P1	123.7(8)	C43	P3	Pd4	115.6(3)
C18	C13	P1	117.6(8)	C49	P3	Pd4	113.0(3)
C13	C14	C15	119.8(12)	C55	P4	Pd1	114.8(3)
C16	C15	C14	120.6(14)	C55	P4	Pd2	111.3(3)
C15	C16	C17	121.6(12)	C55	P4	Pd3	116.8(3)
C16	C17	C18	118.6(13)	C55	P4	S1	106.7(3)
C17	C18	C13	121.0(12)	Pd1	P4	Pd2	63.01(5)
C20	C19	C24	119.2(10)	Pd3	P4	Pd1	71.57(6)
C20	C19	P2	119.4(8)	Pd3	P4	Pd2	123.84(7)
C24	C19	P2	121.3(9)	S1	P4	Pd1	116.69(10)
C19	C20	C21	121.2(13)	S1	P4	Pd2	58.26(7)
C22	C21	C20	120.9(15)	S1	P4	Pd3	126.58(11)
C21	C22	C23	119.5(13)	C60	P5	Pd1	110.8(3)
C22	C23	C24	120.8(15)	C60	P5	Pd3	105.9(3)

C19	C24	C23	118.3(14)	C60	P5	Pd4	120.5(3)
C26	C25	C30	118.7(10)	C60	P5	S2	105.0(3)
C26	C25	P2	121.7(9)	Pd1	P5	Pd3	62.59(5)
C30	C25	P2	119.4(9)	Pd4	P5	Pd1	70.73(6)
C25	C26	C27	119.9(14)	Pd4	P5	Pd3	122.90(8)
C28	C27	C26	118.5(16)	S2	P5	Pd1	116.34(10)
C29	C28	C27	123.7(15)	S2	P5	Pd3	57.78(8)
C28	C29	C30	115.8(16)	S2	P5	Pd4	128.30(11)
C25	C30	C29	123.4(14)	C65	P6	Pd1	116.8(3)
C32	C31	C36	118.3(9)	C65	P6	Pd2	118.5(3)
C32	C31	P2	123.8(8)	C65	P6	Pd4	112.5(3)
C36	C31	P2	117.8(7)	C65	P6	S3	105.7(3)
C31	C32	C33	120.7(12)	Pd1	P6	Pd4	61.70(5)
C34	C33	C32	120.7(13)	Pd2	P6	Pd1	71.87(6)
C33	C34	C35	120.0(10)	Pd2	P6	Pd4	122.07(8)
C34	C35	C36	120.5(11)	S3	P6	Pd1	114.61(10)
C31	C36	C35	119.7(10)	S3	P6	Pd2	126.24(11)
C38	C37	C42	120.0(10)	S3	P6	Pd4	56.95(7)
C38	C37	P3	117.8(8)	P4	Pd1	P5	119.70(7)
C42	C37	P3	122.2(8)	P4	Pd1	Pd2	67.12(5)
C37	C38	C39	121.2(13)	P4	Pd1	Pd3	53.88(5)
C40	C39	C38	116.6(15)	P4	Pd1	Pd4	162.62(5)
C41	C40	C39	123.9(15)	P5	Pd1	Pd2	162.94(5)
C40	C41	C42	119.4(14)	P5	Pd1	Pd3	67.64(5)
C37	C42	C41	118.8(13)	P5	Pd1	Pd4	54.52(5)
C44	C43	P3	123.0(7)	P6	Pd1	P4	118.75(7)
C48	C43	C44	117.8(9)	P6	Pd1	P5	121.54(7)
C48	C43	P3	119.0(7)	P6	Pd1	Pd2	54.00(5)
C45	C44	C43	120.5(10)	P6	Pd1	Pd3	163.42(5)
C46	C45	C44	120.7(11)	P6	Pd1	Pd4	69.22(5)
C45	C46	C47	119.4(10)	Pd3	Pd1	Pd2	112.79(2)
C46	C47	C48	120.8(11)	Pd4	Pd1	Pd2	113.88(2)
C43	C48	C47	120.7(10)	Pd4	Pd1	Pd3	113.82(2)
C50	C49	P3	122.8(7)	P1	Pd2	P4	156.15(7)
C54	C49	C50	118.0(8)	P1	Pd2	Pd1	152.59(6)
C54	C49	P3	119.2(7)	P1	Pd2	S1	110.93(7)
C51	C50	C49	119.4(10)	P6	Pd2	P1	101.60(7)
C52	C51	C50	121.4(11)	P6	Pd2	P4	102.25(6)
C51	C52	C53	119.6(10)	P6	Pd2	Pd1	54.13(5)
C54	C53	C52	119.4(11)	P6	Pd2	S1	146.57(7)

C53	C54	C49	122.2(10)	Pd1	Pd2	P4	49.87(4)
C56	C55	N1	106.0(7)	S1	Pd2	P4	45.47(6)
C56	C55	P4	128.9(7)	S1	Pd2	Pd1	92.45(5)
N1	C55	P4	125.1(6)	P2	Pd3	P5	155.14(7)
C55	C56	C57	108.4(9)	P2	Pd3	Pd1	155.08(6)
C58	C57	C56	108.8(8)	P2	Pd3	S2	111.35(7)
C57	C58	N1	107.2(8)	P4	Pd3	P2	101.40(7)
C61	C60	P5	127.9(7)	P4	Pd3	P5	102.97(6)
N2	C60	C61	107.1(8)	P4	Pd3	Pd1	54.54(5)
N2	C60	P5	124.4(6)	P4	Pd3	S2	146.88(7)
C60	C61	C62	107.8(10)	Pd1	Pd3	P5	49.77(4)
C63	C62	C61	107.7(9)	S2	Pd3	P5	45.13(6)
C62	C63	N2	108.5(9)	S2	Pd3	Pd1	92.35(5)
C66	C65	N3	106.9(7)	P3	Pd4	P6	143.61(7)
C66	C65	P6	129.0(7)	P3	Pd4	Pd1	163.64(6)
N3	C65	P6	124.1(6)	P3	Pd4	S3	99.28(7)
C65	C66	C67	108.7(8)	P5	Pd4	P3	114.08(7)
C68	C67	C66	107.0(8)	P5	Pd4	P6	102.30(6)
C67	C68	N3	109.3(9)	P5	Pd4	Pd1	54.76(5)
C55	N1	C59	127.3(7)	P5	Pd4	S3	145.83(7)
C58	N1	C55	109.6(7)	Pd1	Pd4	P6	49.08(4)
C58	N1	C59	123.1(8)	S3	Pd4	P6	44.59(6)
C65	N3	C69	127.1(7)	S3	Pd4	Pd1	91.07(5)
C68	N3	C65	108.2(8)	P4	S1	Pd2	76.27(8)
C68	N3	C69	124.7(8)	P5	S2	Pd3	77.09(8)
C60	N2	C64	128.1(7)	P6	S3	Pd4	78.46(8)
C63	N2	C60	108.9(8)	Cl2	C70	Cl1	113.4(17)

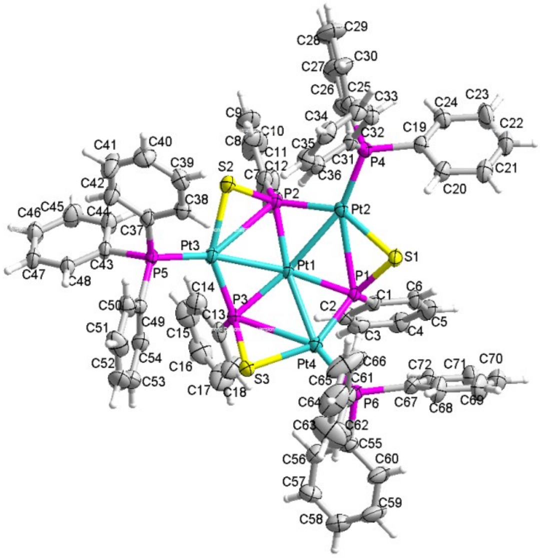
Table 4 Torsion Angles for 2d.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	0.5(16)	C45	C46	C47	C48	0.1(18)
C2	C1	C6	C5	-1.7(15)	C46	C47	C48	C43	-2.8(17)
C2	C1	P1	C7	-177.1(7)	C48	C43	C44	C45	-1.9(14)
C2	C1	P1	C13	76.1(7)	C48	C43	P3	C37	-169.4(7)
C2	C1	P1	Pd2	-55.1(7)	C48	C43	P3	C49	83.3(8)
C2	C3	C4	C5	-0.1(18)	C48	C43	P3	Pd4	-39.2(8)
C3	C4	C5	C6	-1.1(19)	C49	C50	C51	C52	-2.0(19)
C4	C5	C6	C1	2.1(18)	C50	C49	C54	C53	2.1(15)

C6	C1	C2	C3	0.5(14)		C50	C49	P3	C37	-91.9(8)
C6	C1	P1	C7	2.5(9)		C50	C49	P3	C43	15.5(9)
C6	C1	P1	C13	-104.3(8)		C50	C49	P3	Pd4	139.8(7)
C6	C1	P1	Pd2	124.5(7)		C50	C51	C52	C53	3(2)
C7	C8	C9	C10	1.7(18)		C51	C52	C53	C54	-1.0(19)
C8	C7	C12	C11	-0.8(15)		C52	C53	C54	C49	-1.4(17)
C8	C7	P1	C1	86.2(8)		C54	C49	C50	C51	-0.4(15)
C8	C7	P1	C13	-166.8(8)		C54	C49	P3	C37	89.1(8)
C8	C7	P1	Pd2	-36.6(8)		C54	C49	P3	C43	-163.5(7)
C8	C9	C10	C11	-2.7(19)		C54	C49	P3	Pd4	-39.3(8)
C9	C10	C11	C12	1.9(18)		C55	C56	C57	C58	-1.3(12)
C10	C11	C12	C7	-0.2(17)		C56	C55	N1	C58	1.3(10)
C12	C7	C8	C9	0.0(15)		C56	C55	N1	C59	-179.4(9)
C12	C7	P1	C1	-91.5(8)		C56	C55	P4	Pd1	125.7(8)
C12	C7	P1	C13	15.5(9)		C56	C55	P4	Pd2	56.5(9)
C12	C7	P1	Pd2	145.6(7)		C56	C55	P4	Pd3	-153.3(7)
C13	C14	C15	C16	0(2)		C56	C55	P4	S1	-5.3(9)
C14	C13	C18	C17	-0.6(14)		C56	C57	C58	N1	2.1(12)
C14	C13	P1	C1	8.6(9)		C57	C58	N1	C55	-2.2(11)
C14	C13	P1	C7	-98.9(8)		C57	C58	N1	C59	178.5(9)
C14	C13	P1	Pd2	135.9(7)		C60	C61	C62	C63	-1.6(13)
C14	C15	C16	C17	0(2)		C61	C60	N2	C63	0.5(10)
C15	C16	C17	C18	0(2)		C61	C60	N2	C64	178.0(10)
C16	C17	C18	C13	0.3(16)		C61	C60	P5	Pd1	120.2(8)
C18	C13	C14	C15	0.6(15)		C61	C60	P5	Pd3	54.1(9)
C18	C13	P1	C1	-176.7(7)		C61	C60	P5	Pd4	-160.5(8)
C18	C13	P1	C7	75.8(7)		C61	C60	P5	S2	-6.1(9)
C18	C13	P1	Pd2	-49.4(8)		C61	C62	C63	N2	1.9(13)
C19	C20	C21	C22	-2(2)		C62	C63	N2	C60	-1.4(12)

C20	C19	C24	C23	0(2)	C62	C63	N2	C64	-179.1(10)
C20	C19	P2	C25	112.0(10)	C65	C66	C67	C68	-0.4(12)
C20	C19	P2	C31	-139.4(9)	C66	C65	N3	C68	-0.7(10)
C20	C19	P2	Pd3	-9.9(10)	C66	C65	N3	C69	-179.0(9)
C20	C21	C22	C23	4(3)	C66	C65	P6	Pd1	131.1(8)
C21	C22	C23	C24	-5(3)	C66	C65	P6	Pd2	-146.0(7)
C22	C23	C24	C19	3(3)	C66	C65	P6	Pd4	62.5(9)
C24	C19	C20	C21	0(2)	C66	C65	P6	S3	2.3(9)
C24	C19	P2	C25	-66.1(10)	C66	C67	C68	N3	-0.1(12)
C24	C19	P2	C31	42.6(11)	C67	C68	N3	C65	0.5(11)
C24	C19	P2	Pd3	172.1(9)	C67	C68	N3	C69	178.8(10)
C25	C26	C27	C28	-1(3)	N1	C55	C56	C57	0.0(10)
C26	C25	C30	C29	2.3(17)	N1	C55	P4	Pd1	-51.4(7)
C26	C25	P2	C19	-14.7(10)	N1	C55	P4	Pd2	-120.5(6)
C26	C25	P2	C31	-122.7(9)	N1	C55	P4	Pd3	29.6(8)
C26	C25	P2	Pd3	108.5(9)	N1	C55	P4	S1	177.7(6)
C26	C27	C28	C29	1(3)	N3	C65	C66	C67	0.7(11)
C27	C28	C29	C30	1(3)	N3	C65	P6	Pd1	-50.2(8)
C28	C29	C30	C25	-2(2)	N3	C65	P6	Pd2	32.7(8)
C30	C25	C26	C27	-0.7(19)	N3	C65	P6	Pd4	-118.8(7)
C30	C25	P2	C19	171.8(8)	N3	C65	P6	S3	-179.0(6)
C30	C25	P2	C31	63.9(9)	N2	C60	C61	C62	0.7(11)
C30	C25	P2	Pd3	-65.0(8)	N2	C60	P5	Pd1	-49.2(8)
C31	C32	C33	C34	-2(2)	N2	C60	P5	Pd3	-115.4(7)
C32	C31	C36	C35	1.5(14)	N2	C60	P5	Pd4	30.0(9)
C32	C31	P2	C19	-100.0(9)	N2	C60	P5	S2	-175.6(7)
C32	C31	P2	C25	8.6(10)	P1	C1	C2	C3	-179.9(8)

C32	C31	P2	Pd3	133.3(8)	P1	C1	C6	C5	178.7(8)
C32	C33	C34	C35	3(2)	P1	C7	C8	C9	-177.9(9)
C33	C34	C35	C36	-2.0(19)	P1	C7	C12	C11	177.0(8)
C34	C35	C36	C31	-0.5(16)	P1	C13	C14	C15	175.2(9)
C36	C31	C32	C33	-0.1(16)	P1	C13	C18	C17	-175.6(8)
C36	C31	P2	C19	80.8(8)	P2	C19	C20	C21	-178.3(11)
C36	C31	P2	C25	-170.6(7)	P2	C19	C24	C23	177.8(12)
C36	C31	P2	Pd3	-45.9(8)	P2	C25	C26	C27	-174.3(12)
C37	C38	C39	C40	0(2)	P2	C25	C30	C29	175.9(9)
C38	C37	C42	C41	-1.9(19)	P2	C31	C32	C33	-179.3(10)
C38	C37	P3	C43	74.0(9)	P2	C31	C36	C35	-179.3(7)
C38	C37	P3	C49	179.5(9)	P3	C37	C38	C39	179.7(11)
C38	C37	P3	Pd4	-55.0(10)	P3	C37	C42	C41	179.3(11)
C38	C39	C40	C41	1(3)	P3	C43	C44	C45	173.7(8)
C39	C40	C41	C42	-2(3)	P3	C43	C48	C47	-172.1(8)
C40	C41	C42	C37	2(3)	P3	C49	C50	C51	-179.4(9)
C42	C37	C38	C39	0.9(19)	P3	C49	C54	C53	-178.8(8)
C42	C37	P3	C43	-107.1(9)	P4	C55	C56	C57	-177.5(7)
C42	C37	P3	C49	-1.7(10)	P4	C55	N1	C58	179.0(6)
C42	C37	P3	Pd4	123.8(8)	P4	C55	N1	C59	-1.7(12)
C43	C44	C45	C46	-0.7(16)	P5	C60	C61	C62	-170.2(7)
C44	C43	C48	C47	3.6(14)	P5	C60	N2	C63	171.8(7)
C44	C43	P3	C37	15.1(8)	P5	C60	N2	C64	-10.7(14)
C44	C43	P3	C49	-92.2(8)	P6	C65	C66	C67	179.5(7)
C44	C43	P3	Pd4	145.3(7)	P6	C65	N3	C68	-179.6(6)
C44	C45	C46	C47	1.6(17)	P6	C65	N3	C69	2.1(13)



4a

Table 1 Crystal data and structure refinement for 4a.

Empirical formula	$C_{74}H_{64}Cl_4P_6Pt_4S_3$
Formula weight	2157.41
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	15.0406(3)
b/Å	15.4322(3)
c/Å	18.0802(4)
α/°	67.5107(19)
β/°	79.6002(17)
γ/°	78.1335(17)
Volume/Å^3	3770.42(14)
Z	2
ρ_{calc}g/cm^3	1.900
μ/mm^{-1}	17.157
F(000)	2052.0
Crystal size/mm^3	0.16 × 0.08 × 0.07
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.592 to 134.16
Index ranges	-17 ≤ h ≤ 17, -11 ≤ k ≤ 18, -20 ≤ l ≤ 21
Reflections collected	30681
Independent reflections	13463 [R_{int} = 0.0280, R_{sigma} = 0.0328]

Data/restraints/parameters	13463/0/766
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0351, wR_2 = 0.0922
Final R indexes [all data]	R_1 = 0.0413, wR_2 = 0.0959
Largest diff. peak/hole / e $Å^{-3}$	2.59/-1.07

Table 2 Bond Lengths for 4a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.398(10)	C45	C46	1.364(13)
C1	C6	1.386(9)	C46	C47	1.346(13)
C1	P1	1.823(6)	C47	C48	1.382(10)
C2	C3	1.370(10)	C49	C50	1.365(11)
C3	C4	1.375(12)	C49	C54	1.388(11)
C4	C5	1.346(13)	C49	P5	1.848(7)
C5	C6	1.404(11)	C50	C51	1.375(13)
C7	C8	1.371(12)	C51	C52	1.353(16)
C7	C12	1.378(12)	C52	C53	1.393(16)
C7	P2	1.817(8)	C53	C54	1.379(13)
C8	C9	1.419(14)	C55	C56	1.371(11)
C9	C10	1.387(18)	C55	C60	1.371(11)
C10	C11	1.341(17)	C55	P6	1.823(7)
C11	C12	1.390(13)	C56	C57	1.397(12)
C13	C14	1.400(12)	C57	C58	1.351(13)
C13	C18	1.367(12)	C58	C59	1.344(15)
C13	P3	1.830(7)	C59	C60	1.386(14)
C14	C15	1.366(14)	C61	C62	1.366(13)
C15	C16	1.355(16)	C61	C66	1.359(13)
C16	C17	1.353(17)	C61	P6	1.819(8)
C17	C18	1.390(13)	C62	C63	1.409(16)
C19	C20	1.383(10)	C63	C64	1.35(2)
C19	C24	1.373(10)	C64	C65	1.38(2)
C19	P4	1.831(7)	C65	C66	1.361(16)
C20	C21	1.349(11)	C67	C68	1.382(12)
C21	C22	1.356(14)	C67	C72	1.398(12)
C22	C23	1.371(15)	C67	P6	1.840(8)
C23	C24	1.403(12)	C68	C69	1.379(14)
C25	C26	1.379(13)	C69	C70	1.382(18)
C25	C30	1.388(12)	C70	C71	1.376(18)
C25	P4	1.819(7)	C71	C72	1.362(12)

C26	C27	1.367(14)	P1	Pt1	2.2883(15)
C27	C28	1.378(17)	P1	Pt2	2.8289(16)
C28	C29	1.315(18)	P1	Pt4	2.2248(15)
C29	C30	1.393(15)	P1	S1	2.038(2)
C31	C32	1.384(10)	P2	Pt1	2.2753(16)
C31	C36	1.407(9)	P2	Pt2	2.2354(16)
C31	P4	1.807(7)	P2	Pt3	2.8729(16)
C32	C33	1.379(11)	P2	S2	2.041(2)
C33	C34	1.379(13)	P3	Pt1	2.2933(16)
C34	C35	1.351(12)	P3	Pt3	2.2369(17)
C35	C36	1.405(10)	P3	Pt4	2.8569(16)
C37	C38	1.401(10)	P3	S3	2.035(2)
C37	C42	1.382(10)	P4	Pt2	2.2299(16)
C37	P5	1.824(7)	P5	Pt3	2.2328(15)
C38	C39	1.369(11)	P6	Pt4	2.2297(17)
C39	C40	1.351(13)	Pt1	Pt2	2.6838(4)
C40	C41	1.372(14)	Pt1	Pt3	2.6694(3)
C41	C42	1.390(13)	Pt1	Pt4	2.6917(4)
C43	C44	1.390(11)	Pt2	S1	2.3951(16)
C43	C48	1.370(9)	Pt3	S2	2.3786(18)
C43	P5	1.842(7)	Pt4	S3	2.3988(16)
C44	C45	1.412(11)			

Table 3 Bond Angles for 4a.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	P1	117.9(5)	C1	P1	Pt1	113.1(2)
C6	C1	C2	118.8(6)	C1	P1	Pt2	113.0(2)
C6	C1	P1	123.2(6)	C1	P1	Pt4	114.5(2)
C3	C2	C1	121.0(7)	C1	P1	S1	108.5(2)
C2	C3	C4	119.3(8)	Pt1	P1	Pt2	62.21(4)
C5	C4	C3	121.3(7)	Pt4	P1	Pt1	73.21(4)
C4	C5	C6	120.4(8)	Pt4	P1	Pt2	124.15(6)
C1	C6	C5	119.2(8)	S1	P1	Pt1	114.79(8)
C8	C7	C12	118.7(8)	S1	P1	Pt2	56.17(6)
C8	C7	P2	120.7(7)	S1	P1	Pt4	128.06(9)
C12	C7	P2	120.5(6)	C7	P2	Pt1	116.3(3)
C7	C8	C9	120.9(11)	C7	P2	Pt2	117.5(2)
C10	C9	C8	117.7(11)	C7	P2	Pt3	113.9(2)
C11	C10	C9	121.7(10)	C7	P2	S2	107.0(3)
C10	C11	C12	119.8(11)	Pt1	P2	Pt3	61.17(4)

C7	C12	C11	121.1(10)	Pt2	P2	Pt1	73.02(5)
C14	C13	P3	118.7(7)	Pt2	P2	Pt3	121.92(6)
C18	C13	C14	118.0(8)	S2	P2	Pt1	112.51(9)
C18	C13	P3	123.0(7)	S2	P2	Pt2	126.57(10)
C15	C14	C13	120.7(10)	S2	P2	Pt3	54.79(6)
C16	C15	C14	120.2(12)	C13	P3	Pt1	108.3(2)
C17	C16	C15	120.4(11)	C13	P3	Pt3	116.9(3)
C16	C17	C18	120.3(12)	C13	P3	Pt4	111.0(2)
C13	C18	C17	120.3(11)	C13	P3	S3	108.2(3)
C20	C19	P4	118.3(6)	Pt1	P3	Pt4	61.88(4)
C24	C19	C20	118.2(7)	Pt3	P3	Pt1	72.19(5)
C24	C19	P4	123.3(6)	Pt3	P3	Pt4	121.29(7)
C21	C20	C19	121.3(8)	S3	P3	Pt1	115.22(9)
C20	C21	C22	120.8(9)	S3	P3	Pt3	129.02(10)
C21	C22	C23	120.2(8)	S3	P3	Pt4	55.72(6)
C22	C23	C24	119.0(9)	C19	P4	Pt2	115.6(2)
C19	C24	C23	120.4(9)	C25	P4	C19	103.6(3)
C26	C25	C30	117.9(9)	C25	P4	Pt2	115.7(3)
C26	C25	P4	119.2(7)	C31	P4	C19	102.4(3)
C30	C25	P4	122.8(7)	C31	P4	C25	106.8(3)
C27	C26	C25	120.4(11)	C31	P4	Pt2	111.5(2)
C26	C27	C28	121.9(12)	C37	P5	C43	104.0(3)
C29	C28	C27	117.4(11)	C37	P5	C49	103.8(3)
C28	C29	C30	123.6(12)	C37	P5	Pt3	113.0(2)
C25	C30	C29	118.8(12)	C43	P5	C49	102.4(3)
C32	C31	C36	117.8(7)	C43	P5	Pt3	115.3(2)
C32	C31	P4	123.2(5)	C49	P5	Pt3	116.8(2)
C36	C31	P4	119.0(5)	C55	P6	C67	101.2(3)
C33	C32	C31	121.7(8)	C55	P6	Pt4	115.7(2)
C34	C33	C32	119.9(8)	C61	P6	C55	106.0(4)
C35	C34	C33	120.1(8)	C61	P6	C67	103.2(4)
C34	C35	C36	121.0(8)	C61	P6	Pt4	111.9(3)
C35	C36	C31	119.5(7)	C67	P6	Pt4	117.4(2)
C38	C37	P5	119.4(5)	P1	Pt1	P3	119.65(6)
C42	C37	C38	117.6(7)	P1	Pt1	Pt2	68.83(4)
C42	C37	P5	122.9(6)	P1	Pt1	Pt3	159.71(4)
C39	C38	C37	120.4(7)	P1	Pt1	Pt4	52.31(4)
C40	C39	C38	121.4(8)	P2	Pt1	P1	119.63(6)
C39	C40	C41	119.6(9)	P2	Pt1	P3	120.70(6)
C40	C41	C42	120.1(9)	P2	Pt1	Pt2	52.81(4)

C37	C42	C41	120.8(8)	P2	Pt1	Pt3	70.53(4)
C44	C43	P5	116.9(5)	P2	Pt1	Pt4	161.72(5)
C48	C43	C44	120.9(7)	P3	Pt1	Pt2	162.68(4)
C48	C43	P5	122.1(6)	P3	Pt1	Pt3	52.93(4)
C43	C44	C45	116.9(8)	P3	Pt1	Pt4	69.40(4)
C46	C45	C44	120.9(9)	Pt2	Pt1	Pt4	112.682(12)
C47	C46	C45	121.1(8)	Pt3	Pt1	Pt2	113.500(12)
C46	C47	C48	119.7(8)	Pt3	Pt1	Pt4	112.211(12)
C43	C48	C47	120.5(8)	P2	Pt2	P1	101.69(5)
C50	C49	C54	119.6(8)	P2	Pt2	Pt1	54.18(4)
C50	C49	P5	122.5(6)	P2	Pt2	S1	145.77(6)
C54	C49	P5	117.8(6)	P4	Pt2	P1	149.44(5)
C49	C50	C51	121.2(10)	P4	Pt2	P2	108.82(6)
C52	C51	C50	120.1(11)	P4	Pt2	Pt1	158.86(4)
C51	C52	C53	119.6(10)	P4	Pt2	S1	104.58(6)
C54	C53	C52	120.5(11)	Pt1	Pt2	P1	48.96(3)
C53	C54	C49	119.0(10)	S1	Pt2	P1	44.97(5)
C56	C55	C60	117.4(8)	S1	Pt2	Pt1	91.60(4)
C56	C55	P6	119.7(6)	P3	Pt3	P2	101.25(5)
C60	C55	P6	122.8(7)	P3	Pt3	Pt1	54.88(4)
C55	C56	C57	121.6(8)	P3	Pt3	S2	145.26(6)
C58	C57	C56	119.3(10)	P5	Pt3	P2	144.01(6)
C59	C58	C57	120.2(9)	P5	Pt3	P3	114.75(6)
C58	C59	C60	120.7(10)	P5	Pt3	Pt1	163.93(5)
C55	C60	C59	120.8(10)	P5	Pt3	S2	99.67(6)
C62	C61	P6	123.0(8)	Pt1	Pt3	P2	48.31(3)
C66	C61	C62	119.0(10)	S2	Pt3	P2	44.51(5)
C66	C61	P6	118.0(8)	S2	Pt3	Pt1	90.52(4)
C61	C62	C63	121.3(13)	P1	Pt4	P3	101.69(5)
C64	C63	C62	117.3(15)	P1	Pt4	P6	110.11(6)
C63	C64	C65	121.9(13)	P1	Pt4	Pt1	54.48(4)
C66	C65	C64	119.3(14)	P1	Pt4	S3	145.97(6)
C61	C66	C65	121.2(13)	P6	Pt4	P3	148.19(6)
C68	C67	C72	118.5(8)	P6	Pt4	Pt1	160.56(5)
C68	C67	P6	123.6(7)	P6	Pt4	S3	103.71(6)
C72	C67	P6	117.7(6)	Pt1	Pt4	P3	48.71(3)
C69	C68	C67	120.0(11)	S3	Pt4	P3	44.52(5)
C68	C69	C70	120.2(11)	S3	Pt4	Pt1	91.69(4)
C71	C70	C69	120.7(11)	P1	S1	Pt2	78.86(7)
C72	C71	C70	118.9(12)	P2	S2	Pt3	80.70(7)

C71	C72	C67	121.8(10)	P3	S3	Pt4	79.76(7)

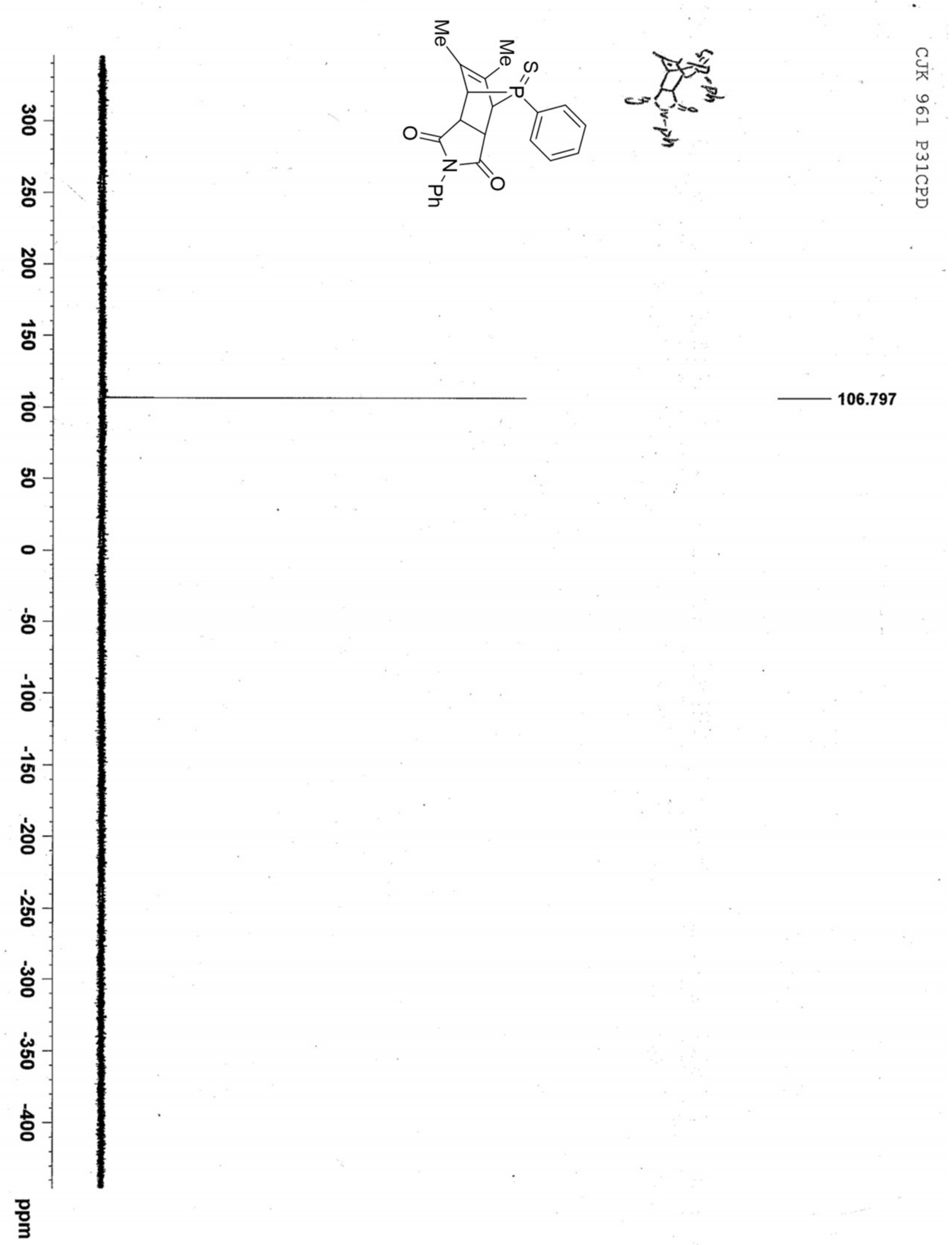
Table 4 Torsion Angles for 4a.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	0.3(12)	C42	C37	P5	C43	10.1(8)
C2	C1	C6	C5	0.8(11)	C42	C37	P5	C49	-96.7(8)
C2	C1	P1	Pt1	-32.2(6)	C42	C37	P5	Pt3	135.8(7)
C2	C1	P1	Pt2	-100.5(5)	C43	C44	C45	C46	-0.6(16)
C2	C1	P1	Pt4	49.2(6)	C44	C43	C48	C47	-0.4(13)
C2	C1	P1	S1	-160.8(5)	C44	C43	P5	C37	91.7(7)
C2	C3	C4	C5	0.3(13)	C44	C43	P5	C49	-160.5(6)
C3	C4	C5	C6	-0.4(14)	C44	C43	P5	Pt3	-32.6(7)
C4	C5	C6	C1	-0.2(12)	C44	C45	C46	C47	-0.4(17)
C6	C1	C2	C3	-0.8(11)	C45	C46	C47	C48	0.9(16)
C6	C1	P1	Pt1	151.9(5)	C46	C47	C48	C43	-0.5(14)
C6	C1	P1	Pt2	83.6(6)	C48	C43	C44	C45	0.9(13)
C6	C1	P1	Pt4	-126.8(5)	C48	C43	P5	C37	-85.1(7)
C6	C1	P1	S1	23.3(6)	C48	C43	P5	C49	22.8(7)
C7	C8	C9	C10	2.2(18)	C48	C43	P5	Pt3	150.7(6)
C8	C7	C12	C11	-1.1(15)	C49	C50	C51	C52	-1.6(16)
C8	C7	P2	Pt1	171.7(7)	C50	C49	C54	C53	-1.6(12)
C8	C7	P2	Pt2	-104.7(7)	C50	C49	P5	C37	5.2(7)
C8	C7	P2	Pt3	103.4(7)	C50	C49	P5	C43	-102.8(6)
C8	C7	P2	S2	44.9(8)	C50	C49	P5	Pt3	130.3(6)

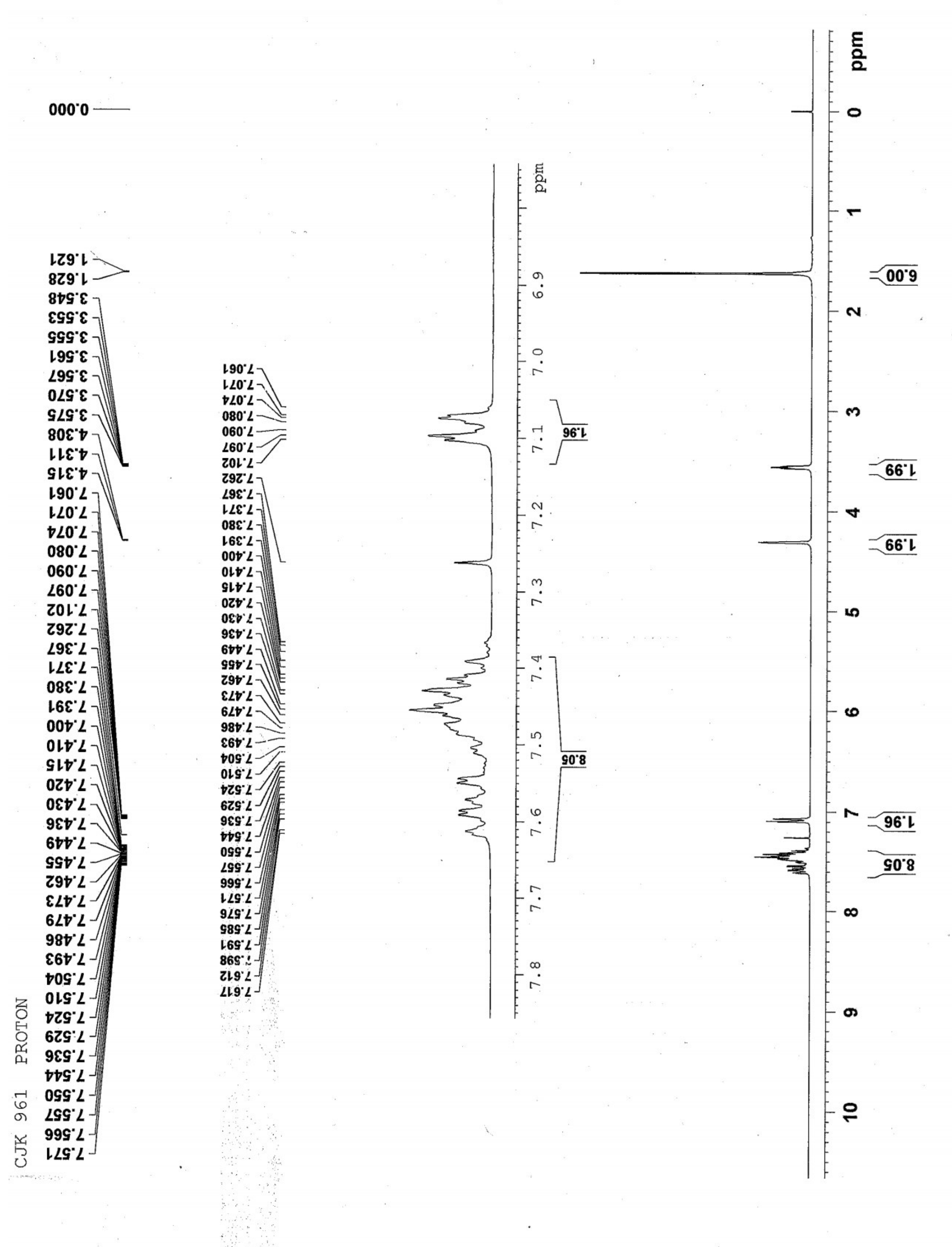
C8	C9	C10	C11	-3(2)	C50	C51	C52	C53	0.4(18)
C9	C10	C11	C12	2(2)	C51	C52	C53	C54	0.2(17)
C10	C11	C12	C7	0.2(18)	C52	C53	C54	C49	0.5(15)
C12	C7	C8	C9	-0.1(15)	C54	C49	C50	C51	2.2(13)
C12	C7	P2	Pt1	-13.4(8)	C54	C49	P5	C37	-178.9(6)
C12	C7	P2	Pt2	70.2(8)	C54	C49	P5	C43	73.1(6)
C12	C7	P2	Pt3	-81.8(7)	C54	C49	P5	Pt3	-53.9(6)
C12	C7	P2	S2	-140.2(7)	C55	C56	C57	C58	-0.9(16)
C13	C14	C15	C16	0.1(17)	C56	C55	C60	C59	-2.6(16)
C14	C13	C18	C17	-1.9(16)	C56	C55	P6	C61	109.5(7)
C14	C13	P3	Pt1	-74.4(6)	C56	C55	P6	C67	-143.1(7)
C14	C13	P3	Pt3	4.4(7)	C56	C55	P6	Pt4	-15.1(7)
C14	C13	P3	Pt4	-140.5(6)	C56	C57	C58	C59	-0.7(18)
C14	C13	P3	S3	160.1(6)	C57	C58	C59	C60	1(2)
C14	C15	C16	C17	-0.6(19)	C58	C59	C60	C55	1(2)
C15	C16	C17	C18	0(2)	C60	C55	C56	C57	2.5(14)
C16	C17	C18	C13	1.3(19)	C60	C55	P6	C61	-74.8(8)
C18	C13	C14	C15	1.2(14)	C60	C55	P6	C67	32.6(9)
C18	C13	P3	Pt1	99.0(8)	C60	C55	P6	Pt4	160.6(7)
C18	C13	P3	Pt3	177.8(7)	C61	C62	C63	C64	-3(3)
C18	C13	P3	Pt4	32.9(9)	C62	C61	C66	C65	-1.2(18)
C18	C13	P3	S3	-26.5(9)	C62	C61	P6	C55	-1.3(10)
C19	C20	C21	C22	-1.1(15)	C62	C61	P6	C67	-107.2(10)
C20	C19	C24	C23	-2.6(14)	C62	C61	P6	Pt4	125.6(9)
C20	C19	P4	C25	169.5(6)	C62	C63	C64	C65	1(3)
C20	C19	P4	C31	58.6(7)	C63	C64	C65	C66	1(3)
C20	C19	P4	Pt2	-62.9(6)	C64	C65	C66	C61	-1(2)
C20	C21	C22	C23	-1.2(17)	C66	C61	C62	C63	3(2)
C21	C22	C23	C24	1.5(18)	C66	C61	P6	C55	176.9(8)
C22	C23	C24	C19	0.4(17)	C66	C61	P6	C67	71.0(8)
C24	C19	C20	C21	2.9(13)	C66	C61	P6	Pt4	-56.2(9)
C24	C19	P4	C25	-15.8(8)	C67	C68	C69	C70	0(2)
C24	C19	P4	C31	-126.7(7)	C68	C67	C72	C71	0.3(14)
C24	C19	P4	Pt2	111.9(7)	C68	C67	P6	C55	-100.8(8)
C25	C26	C27	C28	-2.0(18)	C68	C67	P6	C61	8.8(9)
C26	C25	C30	C29	0.2(16)	C68	C67	P6	Pt4	132.4(7)
C26	C25	P4	C19	88.6(7)	C68	C69	C70	C71	0(2)
C26	C25	P4	C31	-163.7(7)	C69	C70	C71	C72	0(2)
C26	C25	P4	Pt2	-38.9(7)	C70	C71	C72	C67	-0.5(16)
C26	C27	C28	C29	3(2)	C72	C67	C68	C69	-0.2(15)

C27	C28	C29	C30	-3(2)	C72	C67	P6	C55	74.3(7)
C28	C29	C30	C25	1(2)	C72	C67	P6	C61	-176.2(6)
C30	C25	C26	C27	0.3(15)	C72	C67	P6	Pt4	-52.6(7)
C30	C25	P4	C19	-86.3(8)	P1	C1	C2	C3	-176.9(6)
C30	C25	P4	C31	21.4(9)	P1	C1	C6	C5	176.7(6)
C30	C25	P4	Pt2	146.2(7)	P2	C7	C8	C9	174.9(8)
C31	C32	C33	C34	2.4(13)	P2	C7	C12	C11	-176.1(8)
C32	C31	C36	C35	0.0(11)	P3	C13	C14	C15	174.9(8)
C32	C31	P4	C19	34.4(7)	P3	C13	C18	C17	-175.3(9)
C32	C31	P4	C25	-74.1(7)	P4	C19	C20	C21	177.9(7)
C32	C31	P4	Pt2	158.6(6)	P4	C19	C24	C23	-177.3(8)
C32	C33	C34	C35	-2.6(14)	P4	C25	C26	C27	-174.8(8)
C33	C34	C35	C36	1.5(14)	P4	C25	C30	C29	175.2(10)
C34	C35	C36	C31	-0.2(13)	P4	C31	C32	C33	179.6(7)
C36	C31	C32	C33	-1.1(12)	P4	C31	C36	C35	179.3(6)
C36	C31	P4	C19	-144.9(6)	P5	C37	C38	C39	178.6(6)
C36	C31	P4	C25	106.6(6)	P5	C37	C42	C41	-179.2(9)
C36	C31	P4	Pt2	-20.7(6)	P5	C43	C44	C45	-175.8(7)
C37	C38	C39	C40	-0.5(13)	P5	C43	C48	C47	176.2(7)
C38	C37	C42	C41	-2.1(15)	P5	C49	C50	C51	178.0(7)
C38	C37	P5	C43	-167.0(6)	P5	C49	C54	C53	-177.6(7)
C38	C37	P5	C49	86.2(6)	P6	C55	C56	C57	178.4(7)
C38	C37	P5	Pt3	-41.2(6)	P6	C55	C60	C59	-178.4(10)
C38	C39	C40	C41	0.2(16)	P6	C61	C62	C63	-178.7(12)
C39	C40	C41	C42	-0.9(19)	P6	C61	C66	C65	-179.5(10)
C40	C41	C42	C37	1.9(19)	P6	C67	C68	C69	174.8(9)
C42	C37	C38	C39	1.4(12)	P6	C67	C72	C71	-175.0(8)

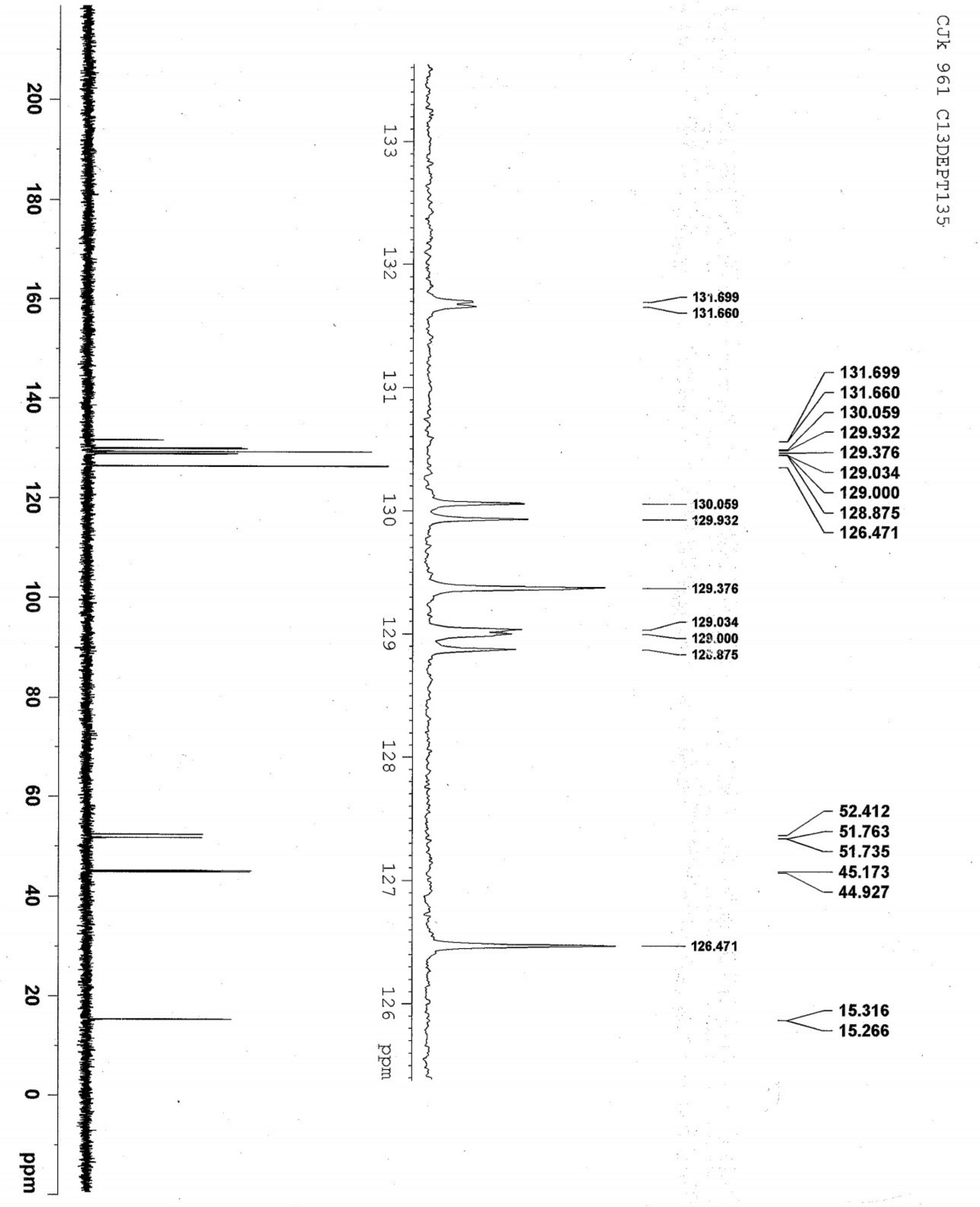
NMR Spectra



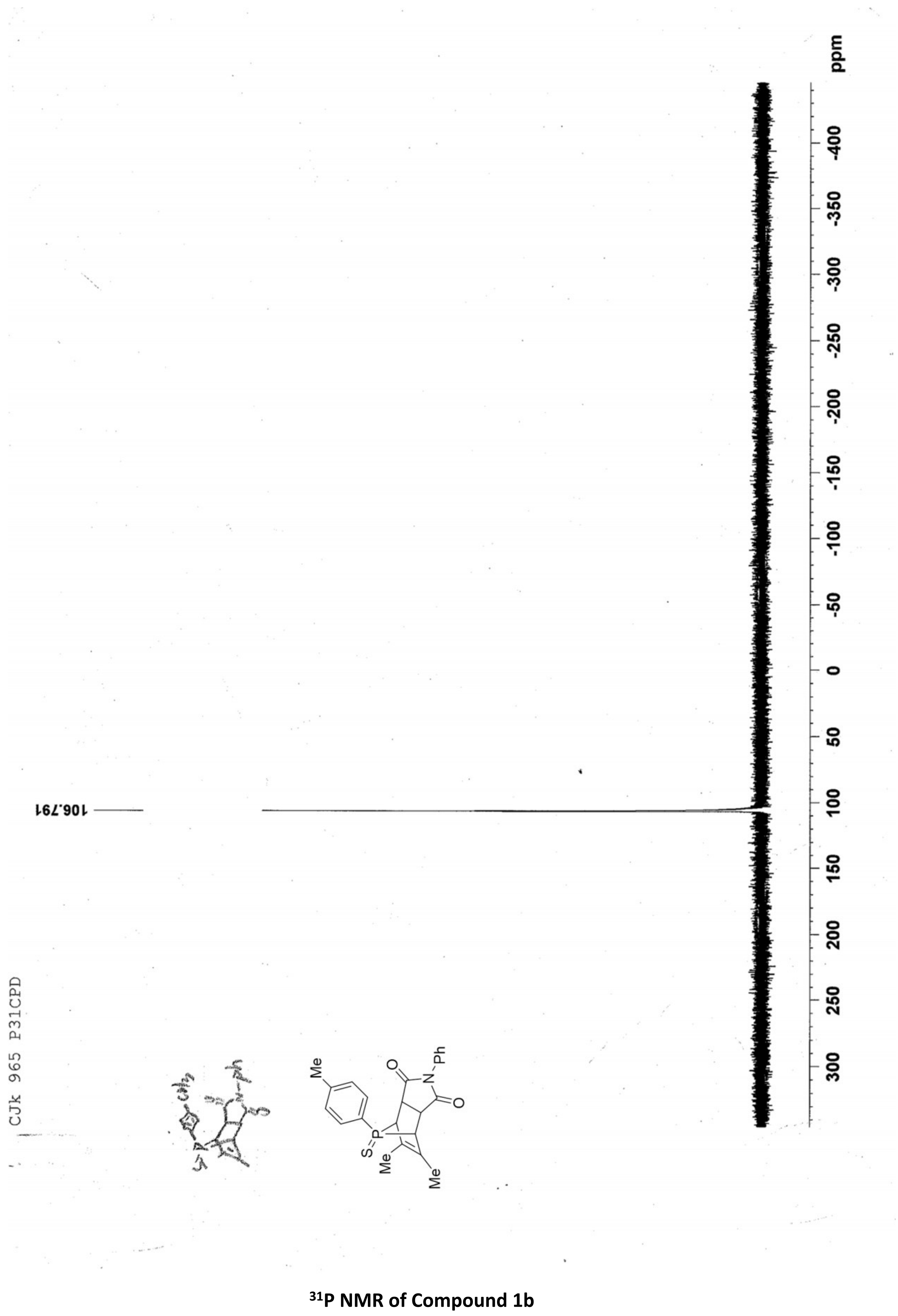
^{31}P NMR of Compound 1a



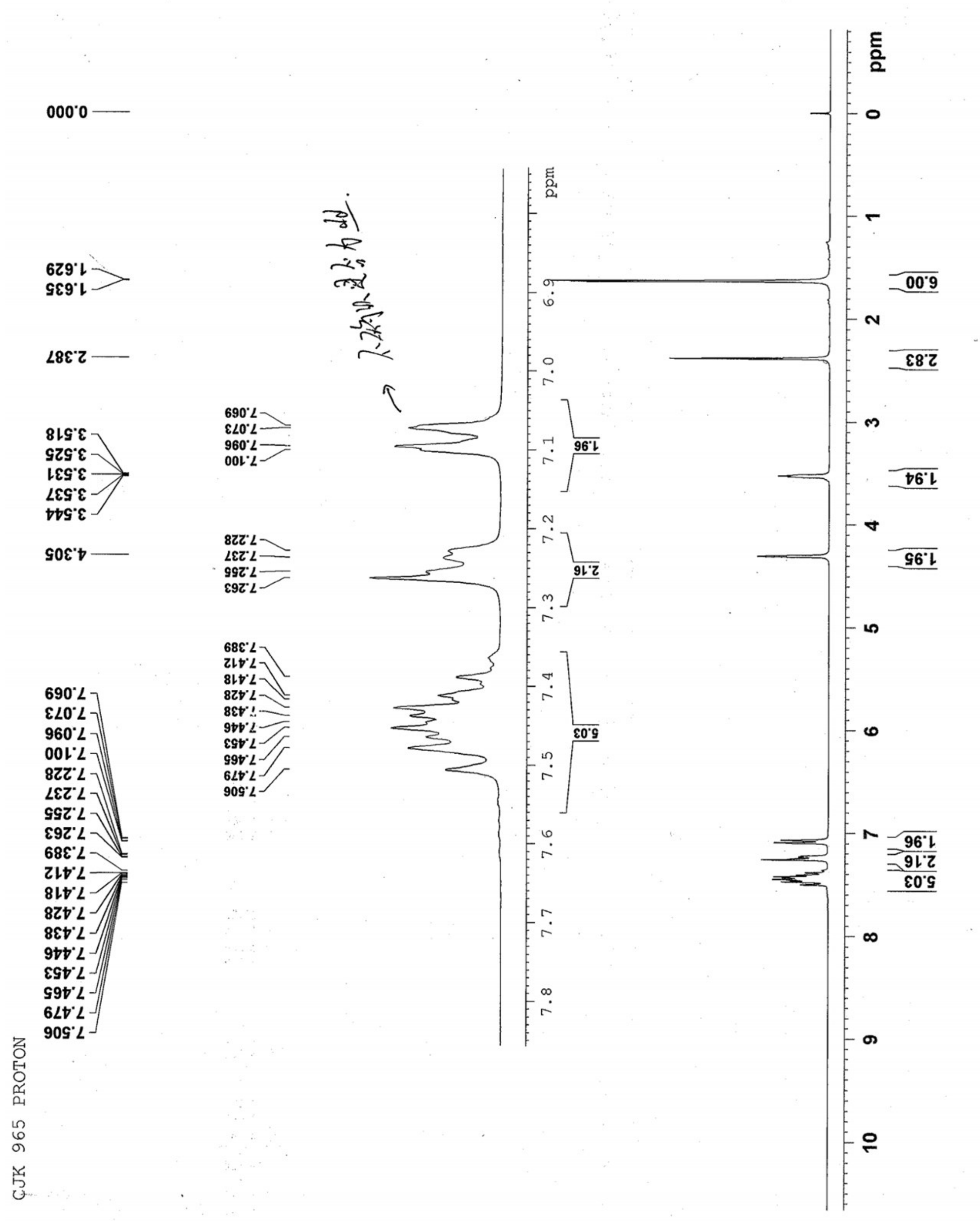
^{1}H NMR of Compound 1a



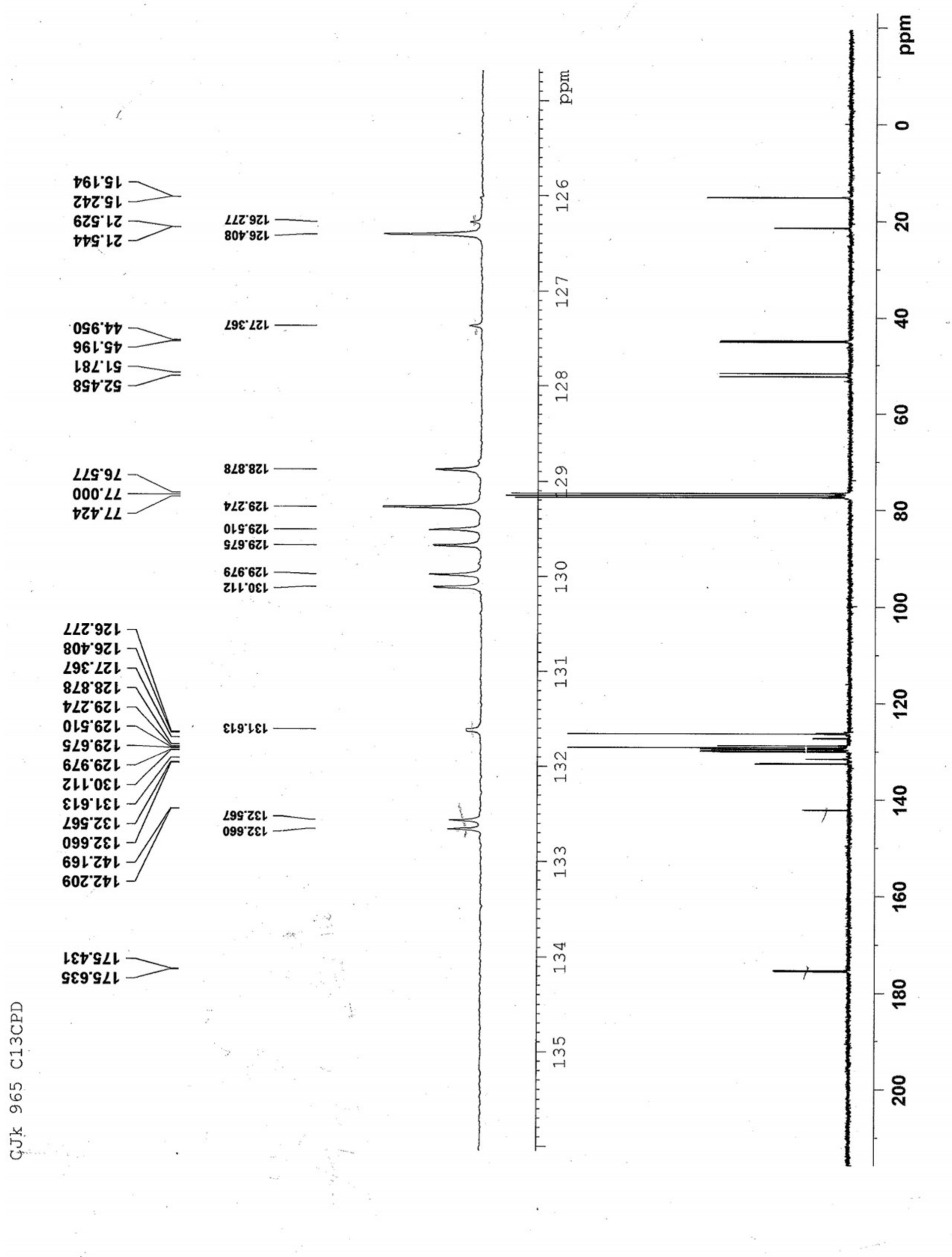
^{13}C NMR of Compound 1a



^{31}P NMR of Compound 1b



^{1}H NMR of Compound 1b



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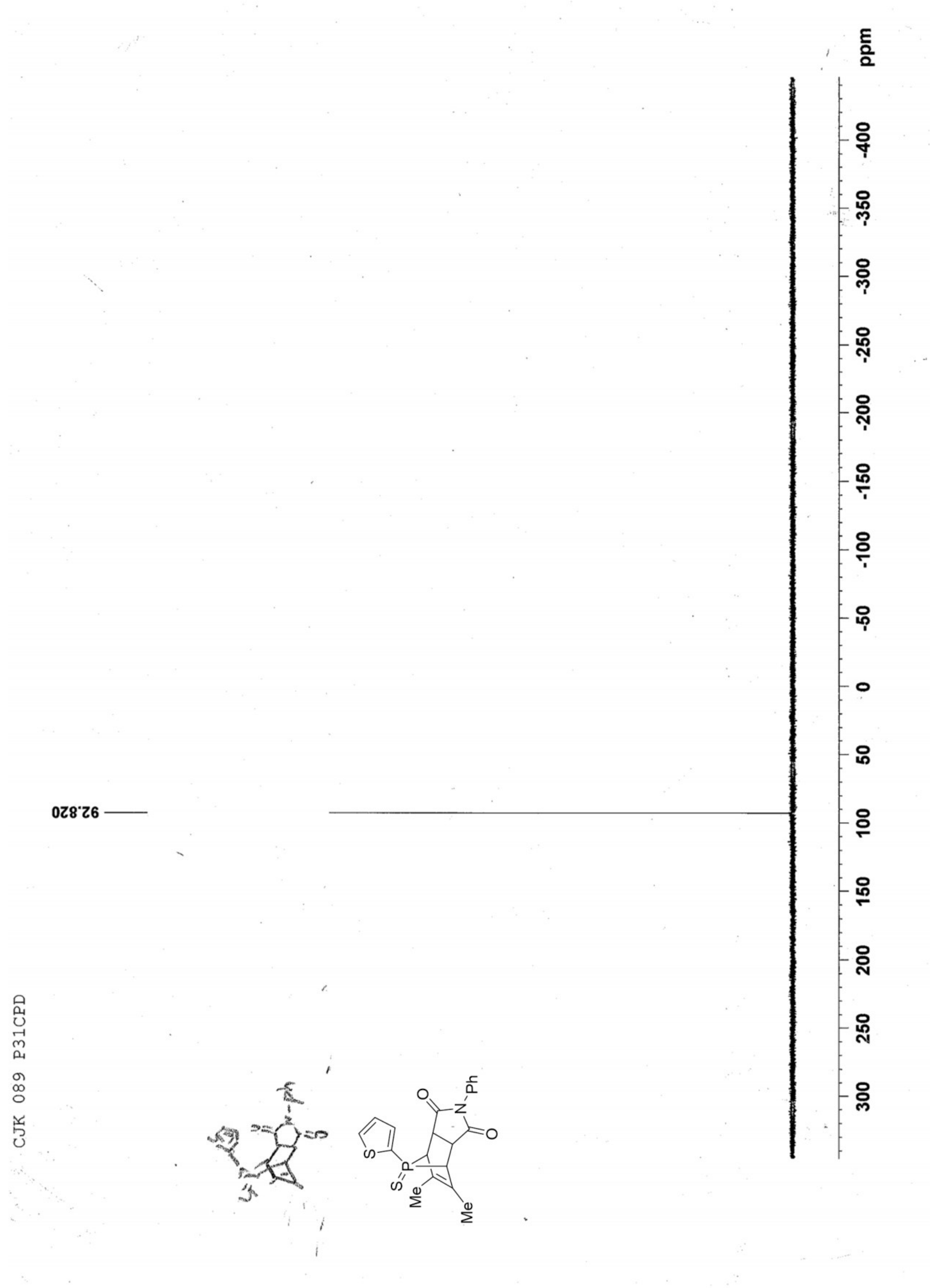
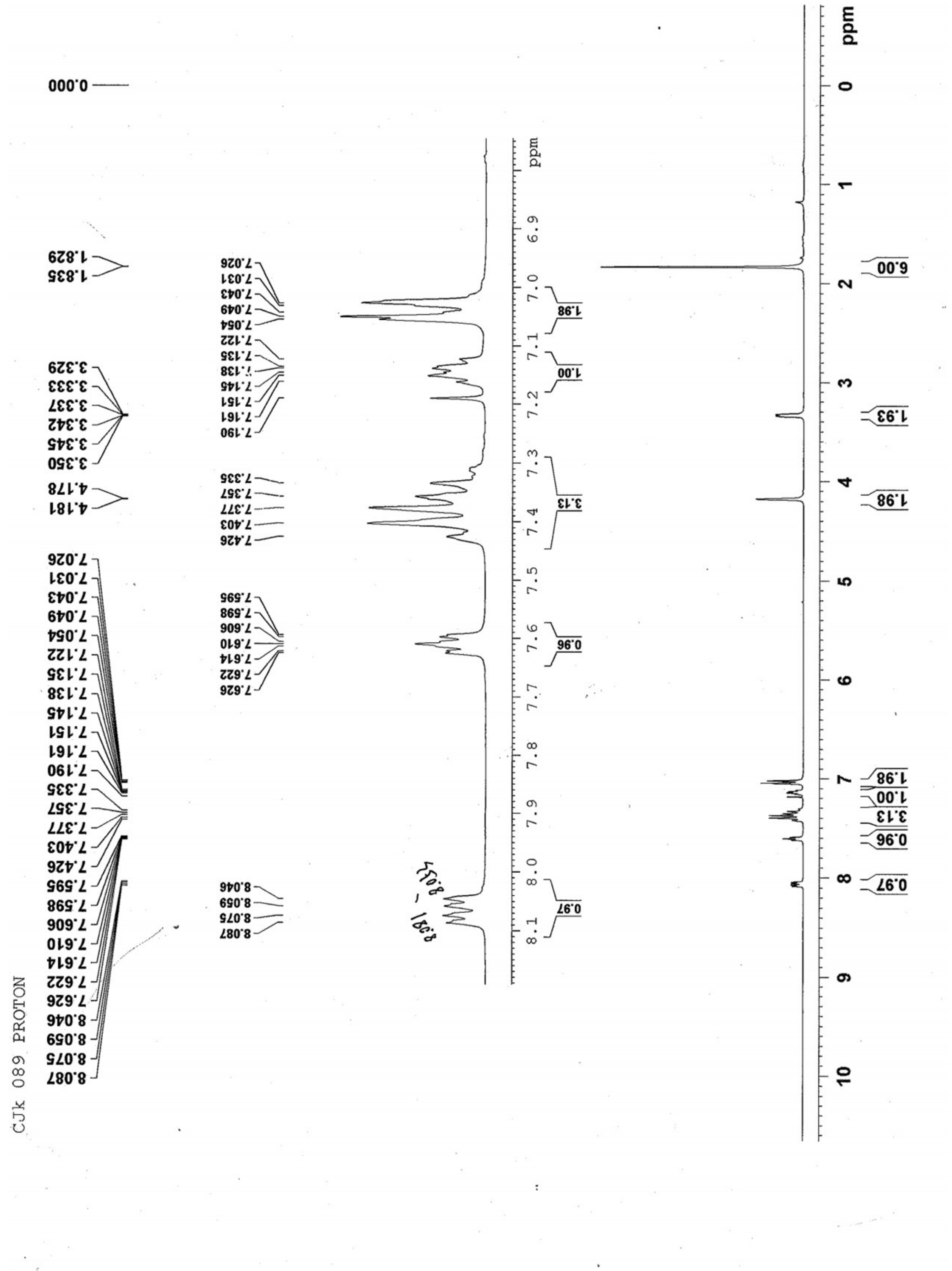


^{31}P NMR of Compound 1c



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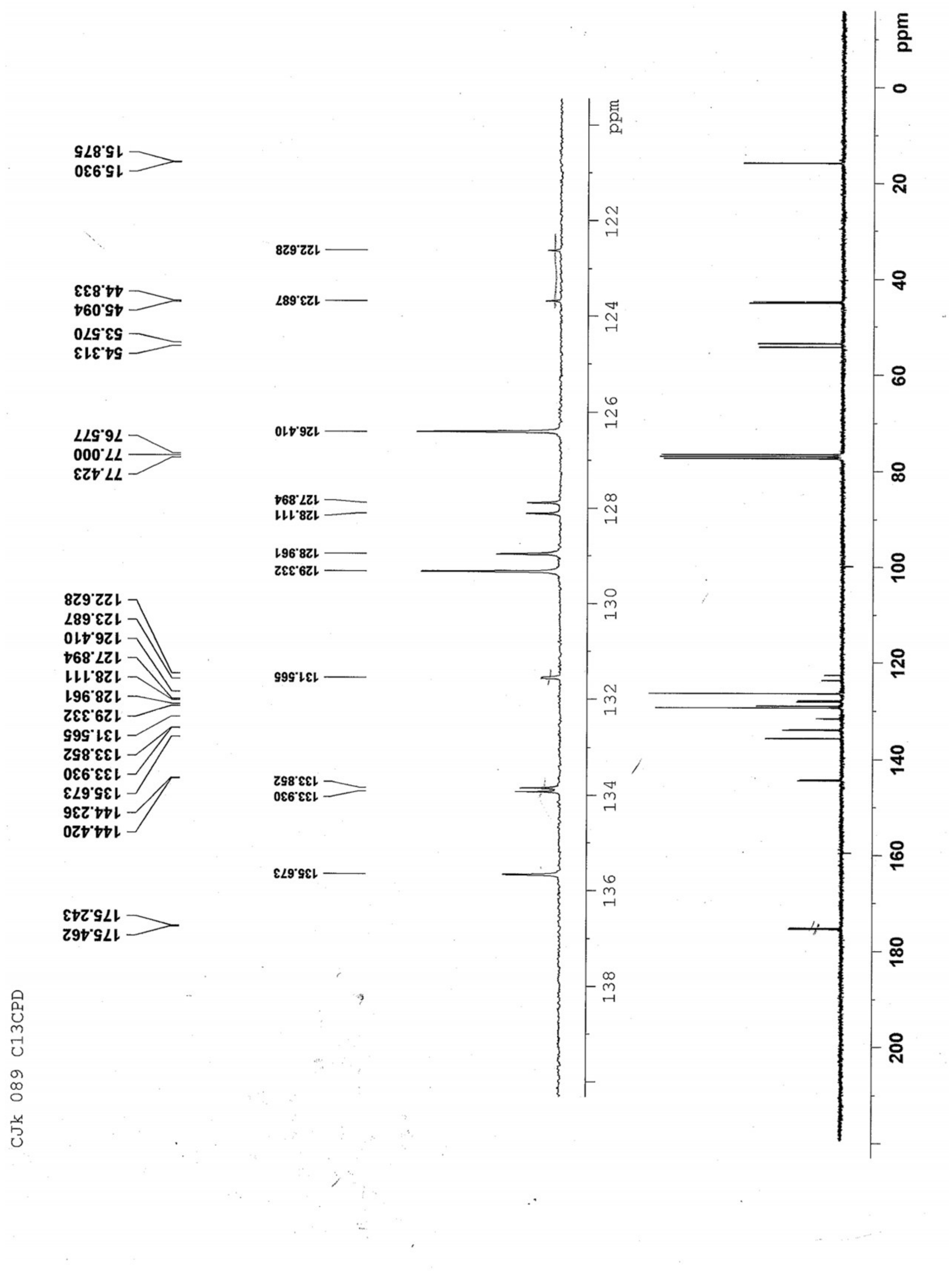

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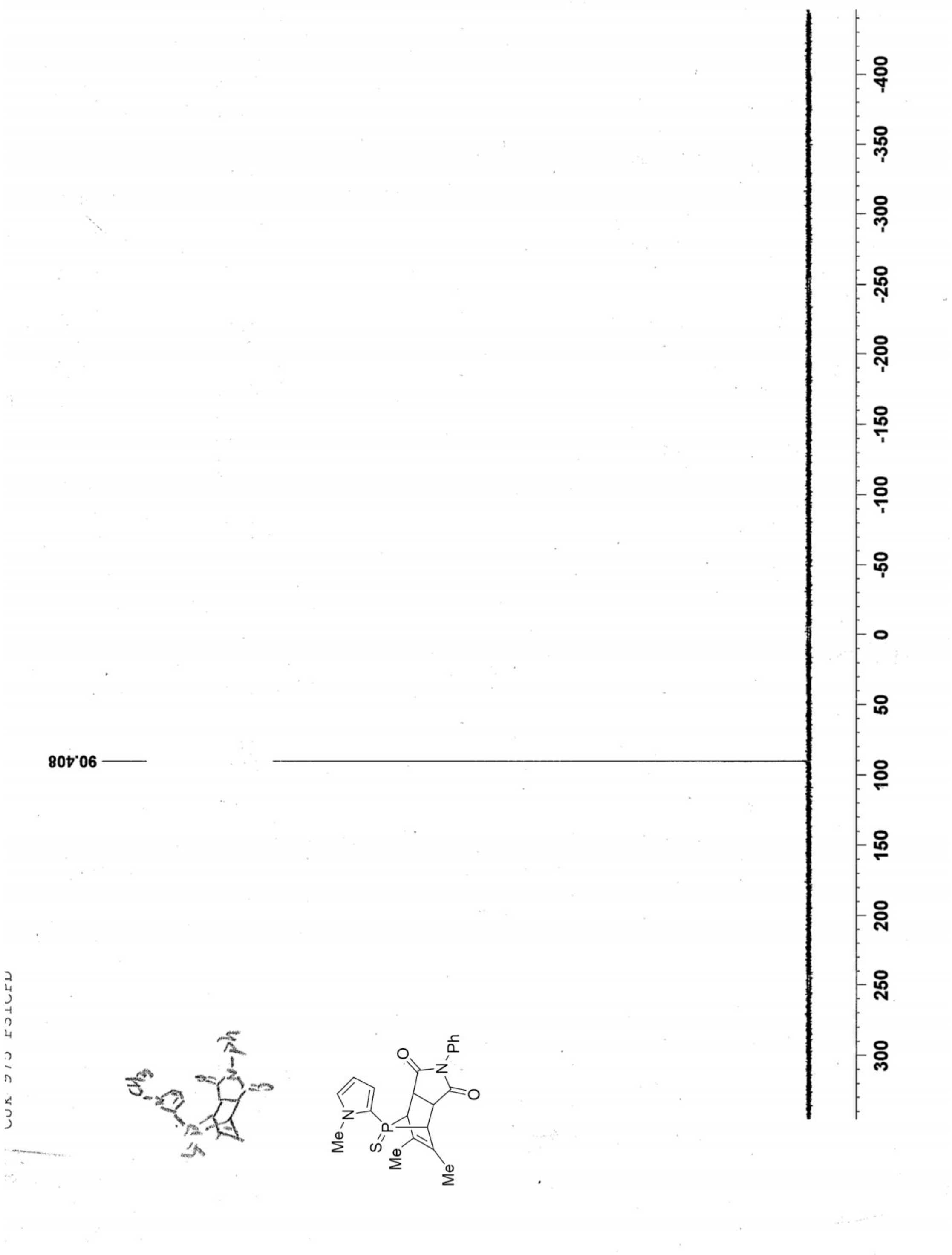
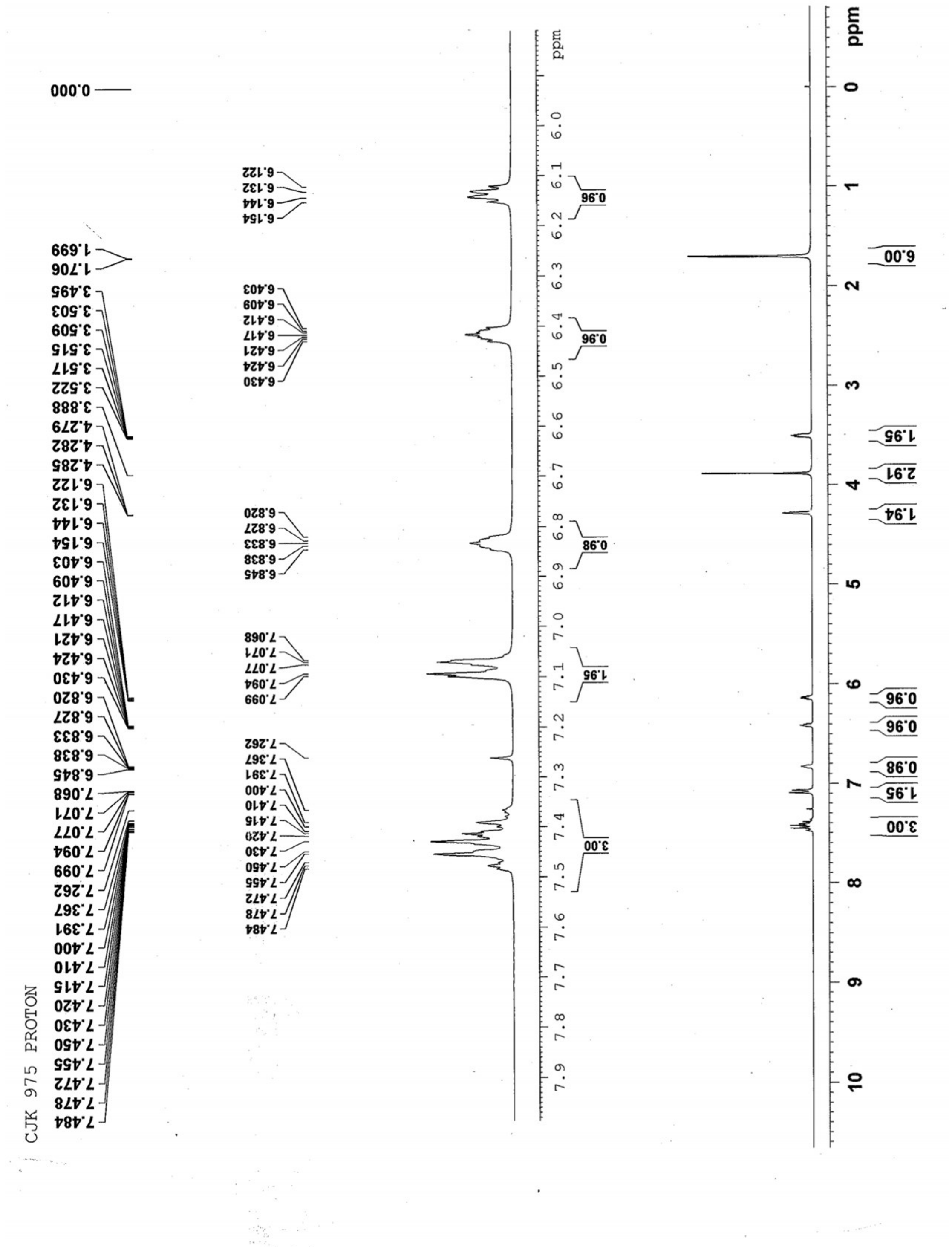


^{31}P NMR of Compound 1d



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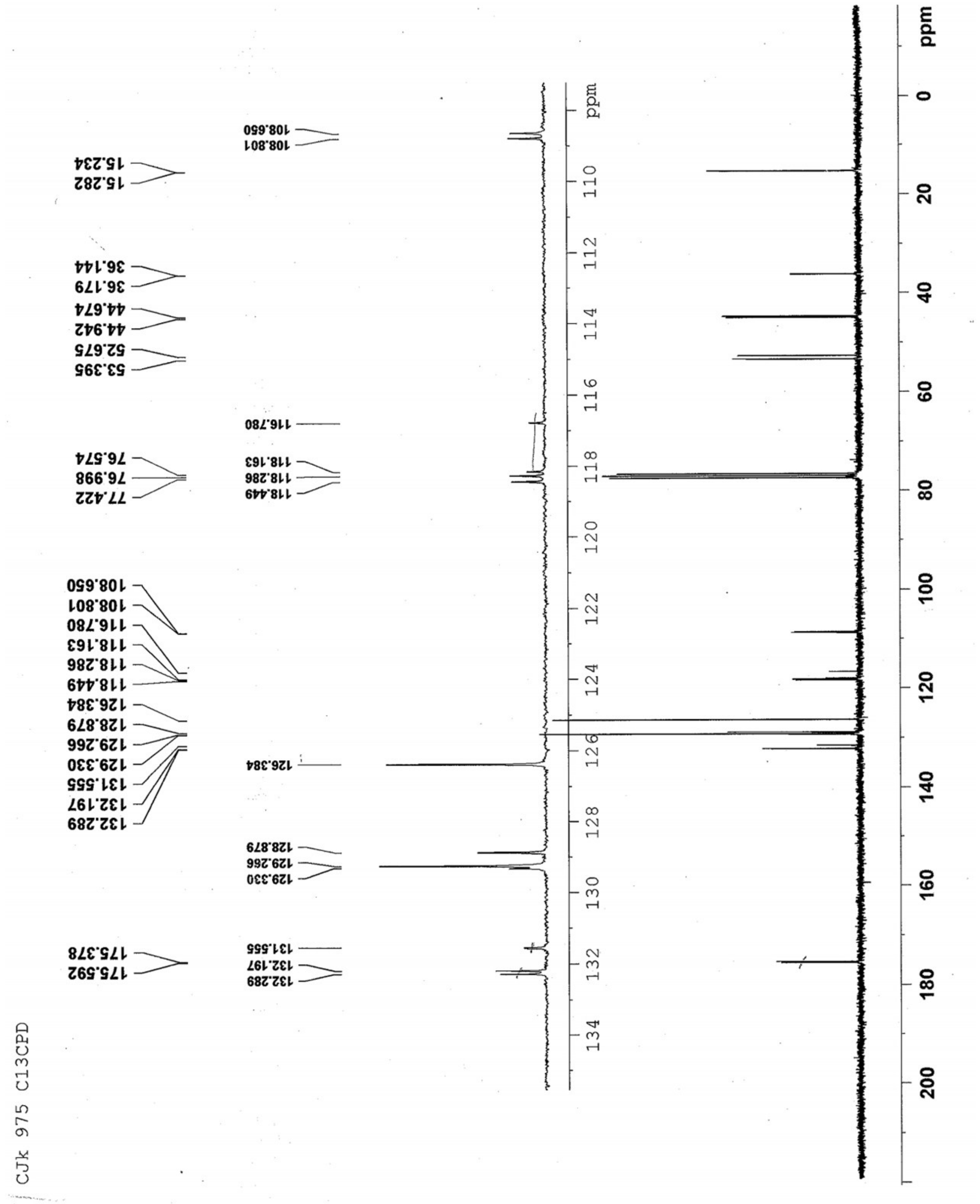

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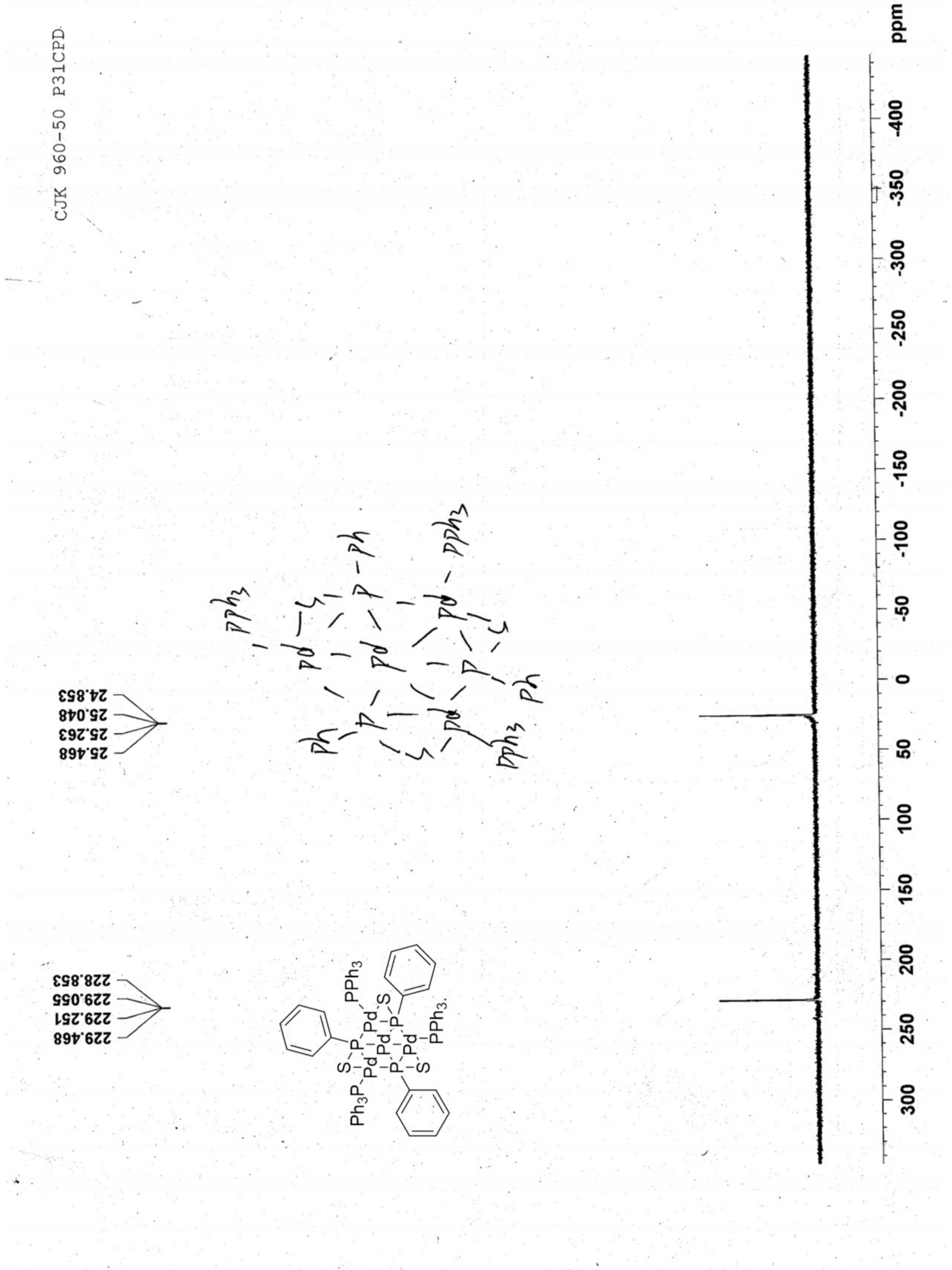
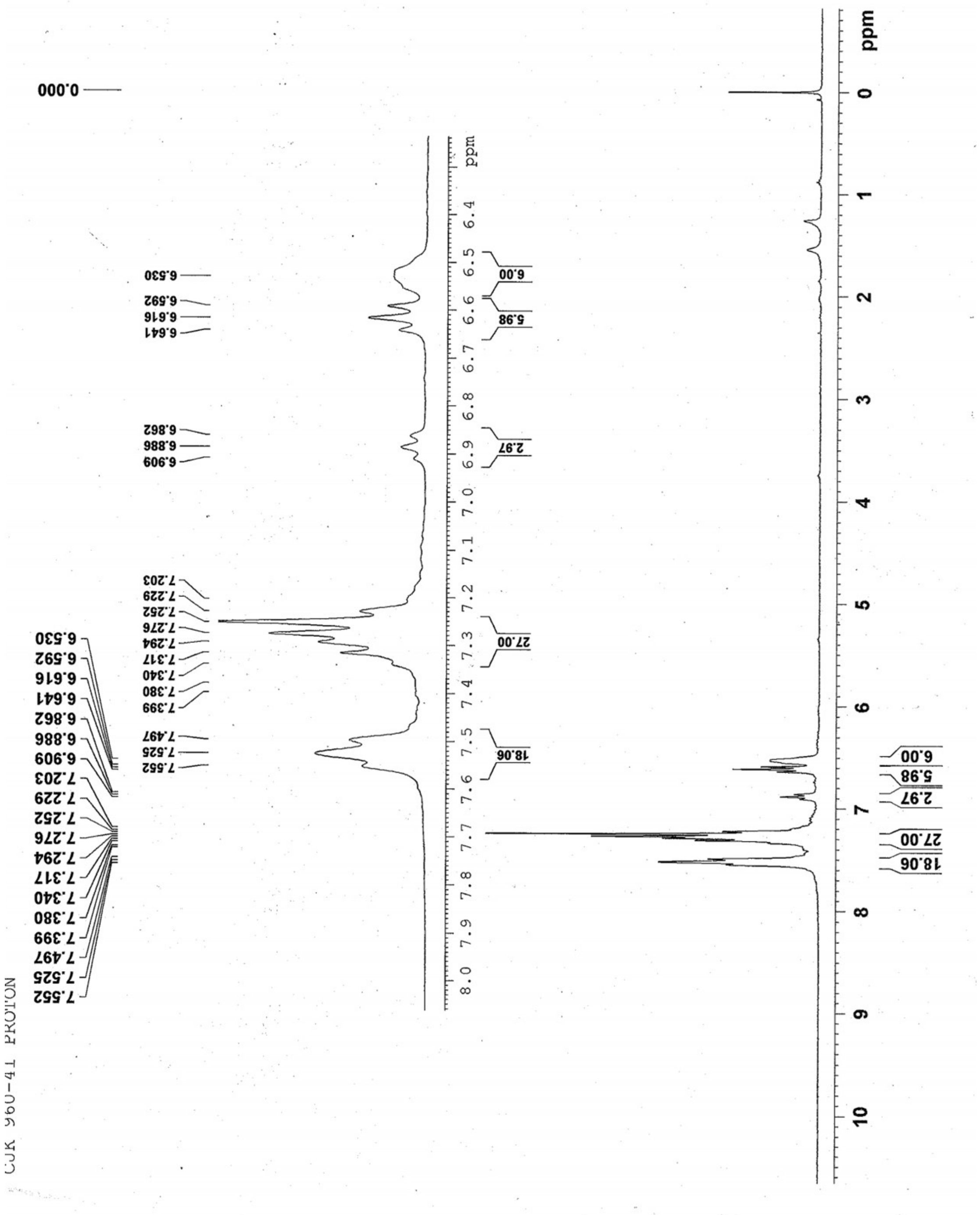
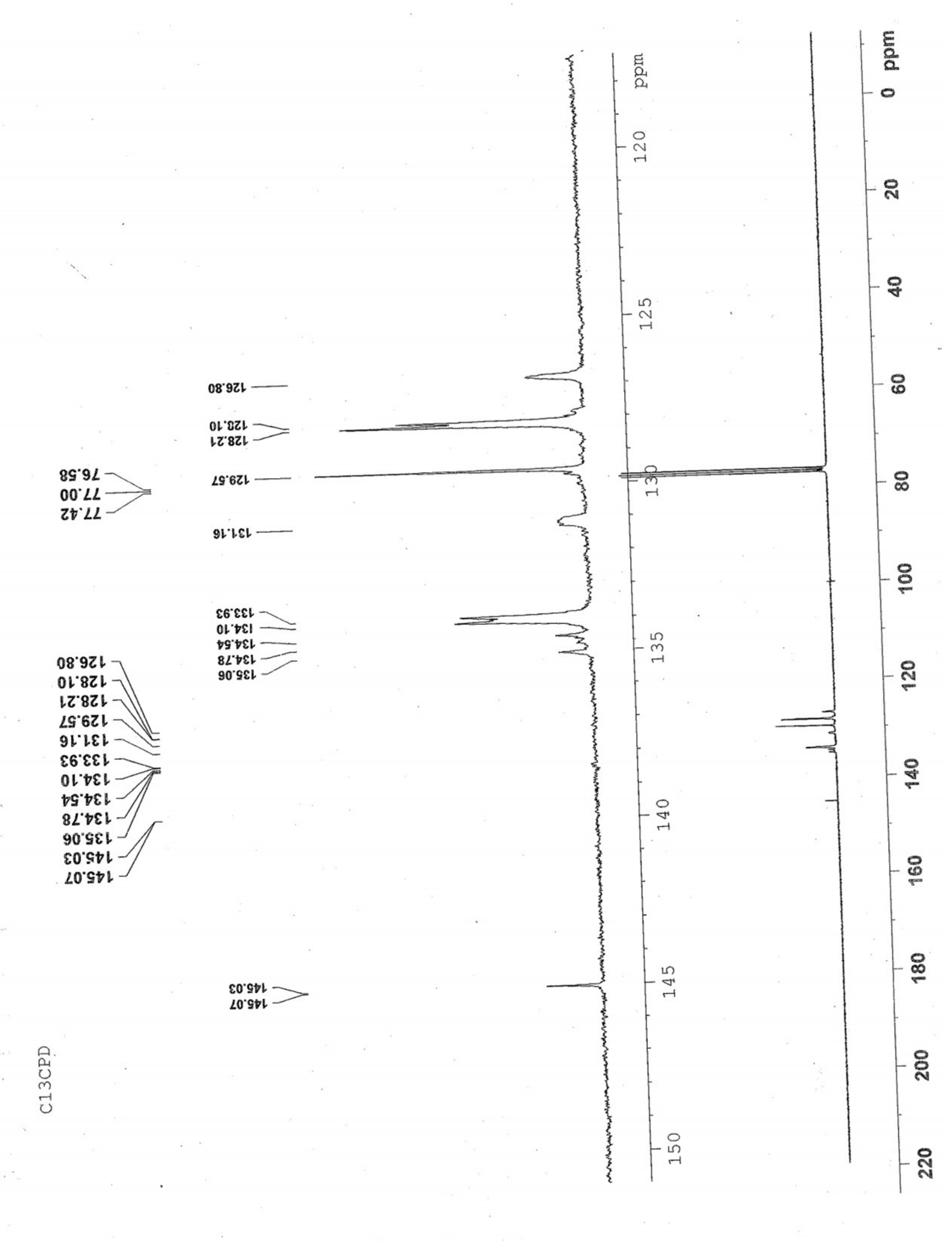


^{31}P NMR of Compound 2a



¹H NMR of Compound 2a



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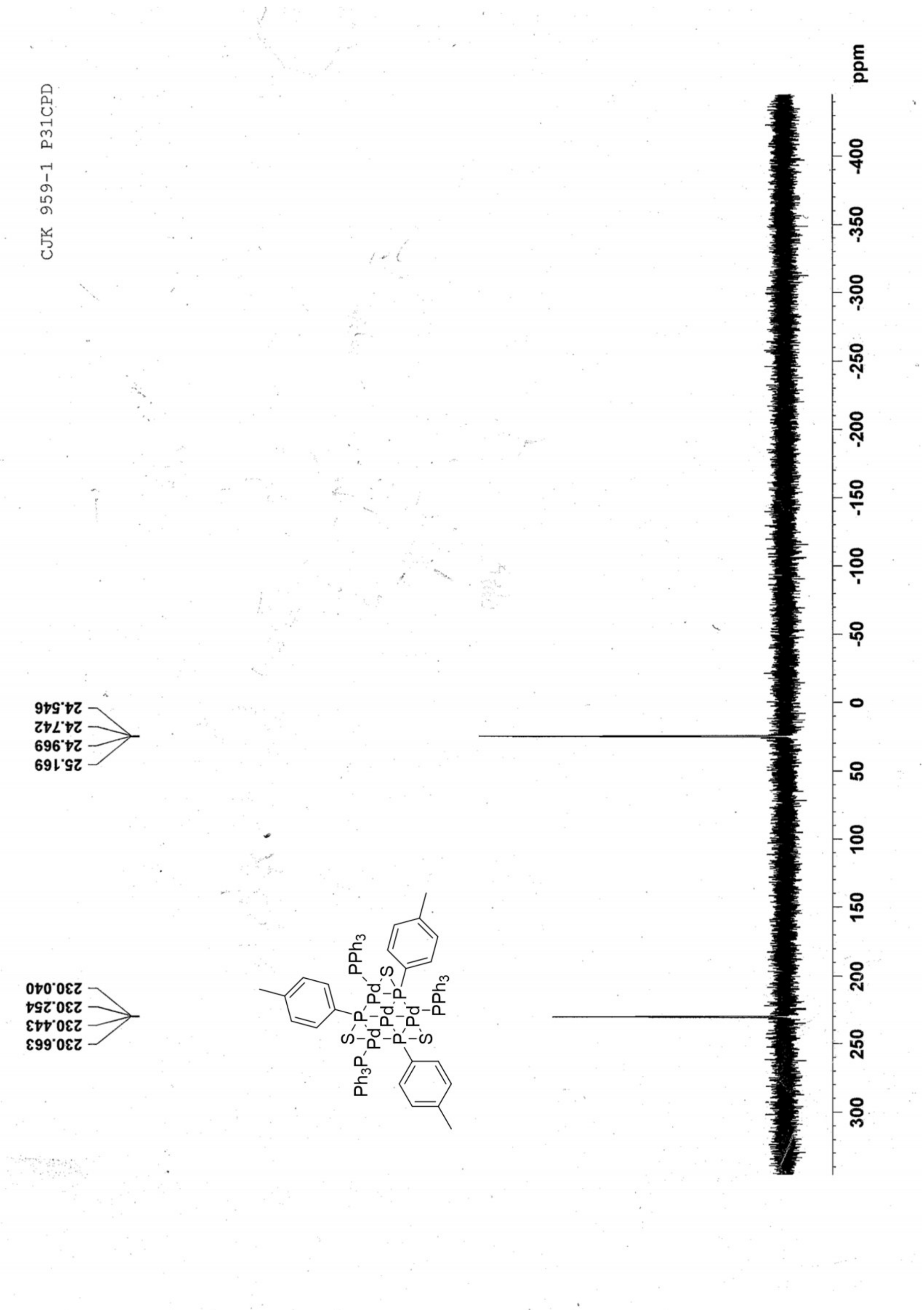
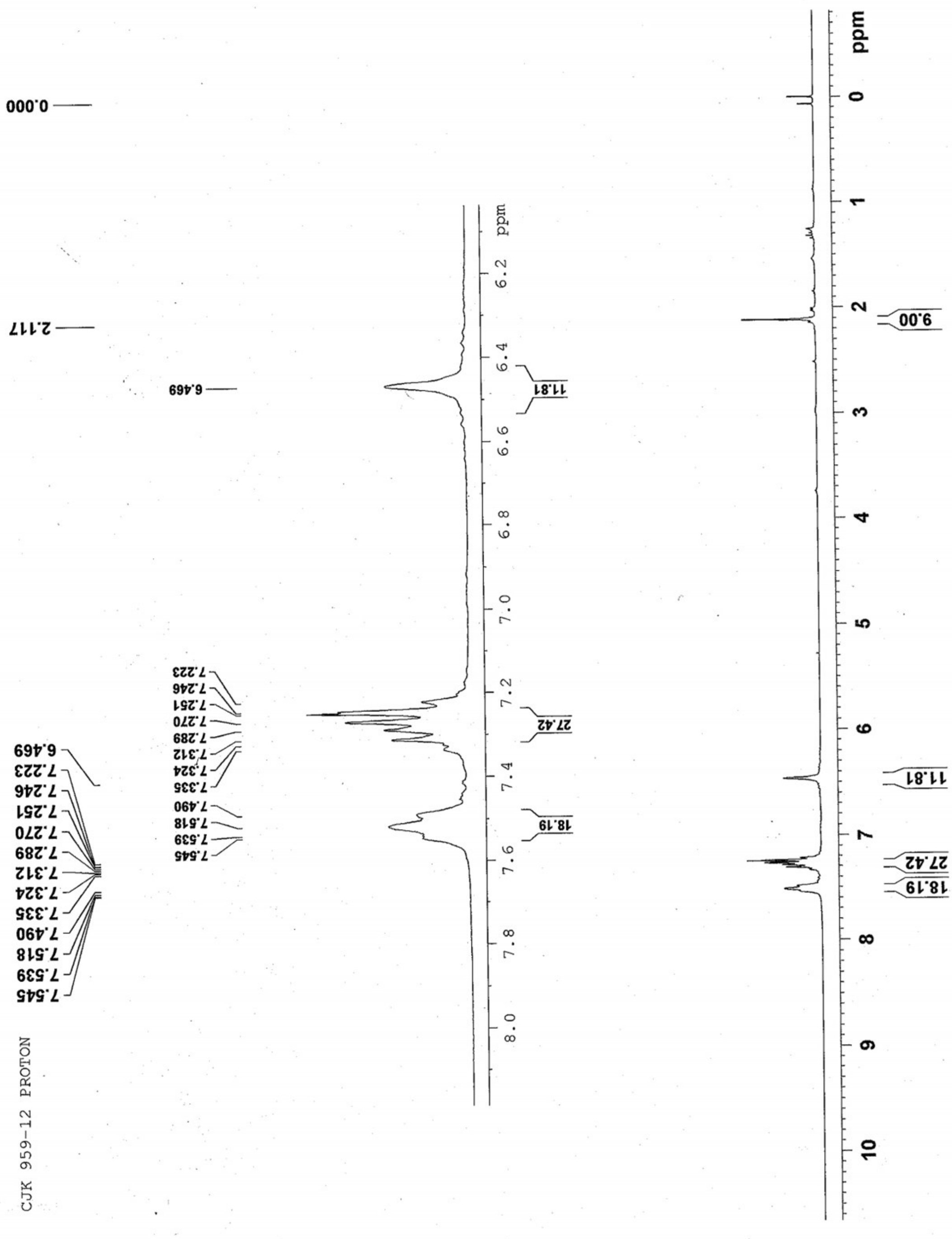


^{31}P NMR of Compound 2b



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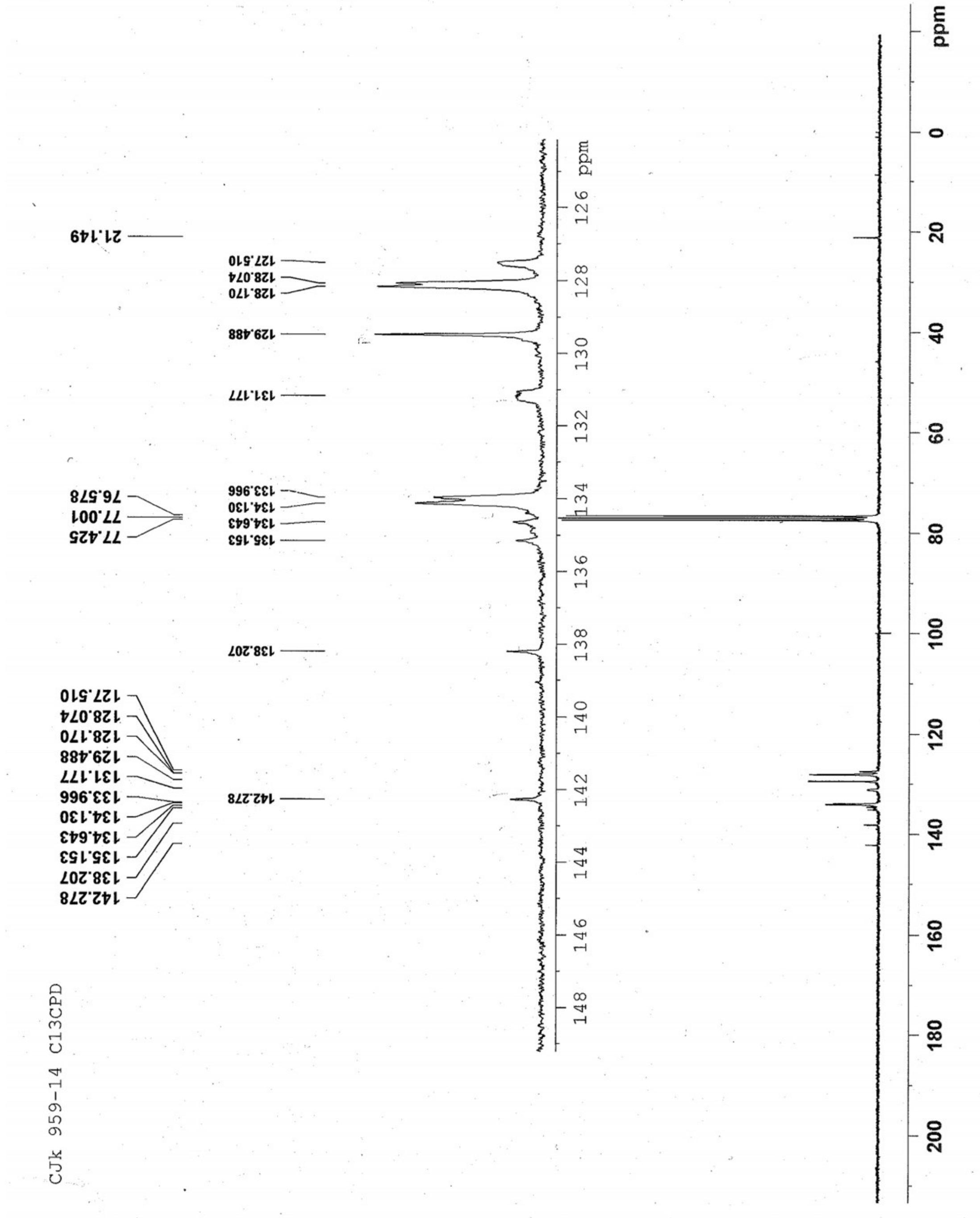

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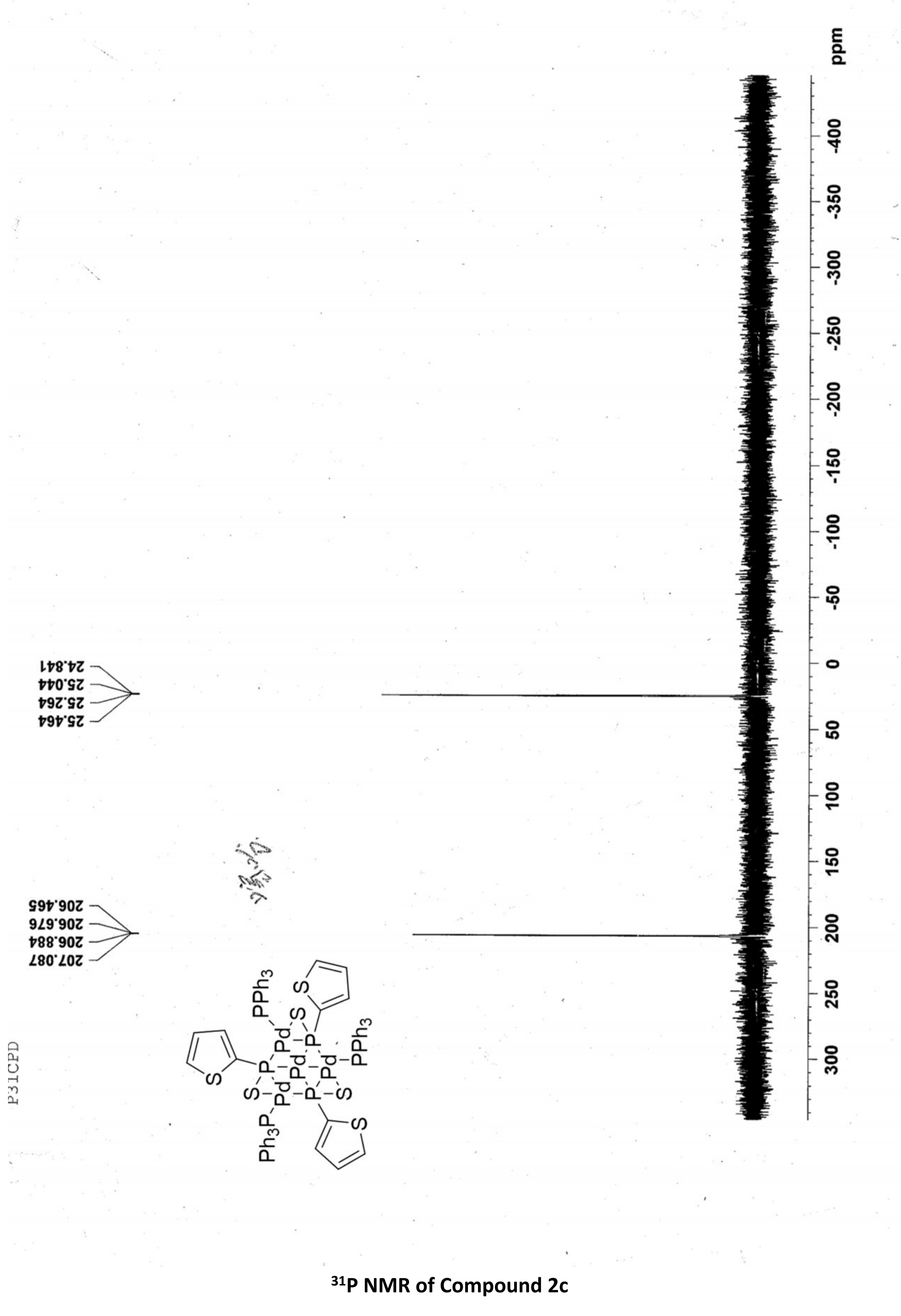
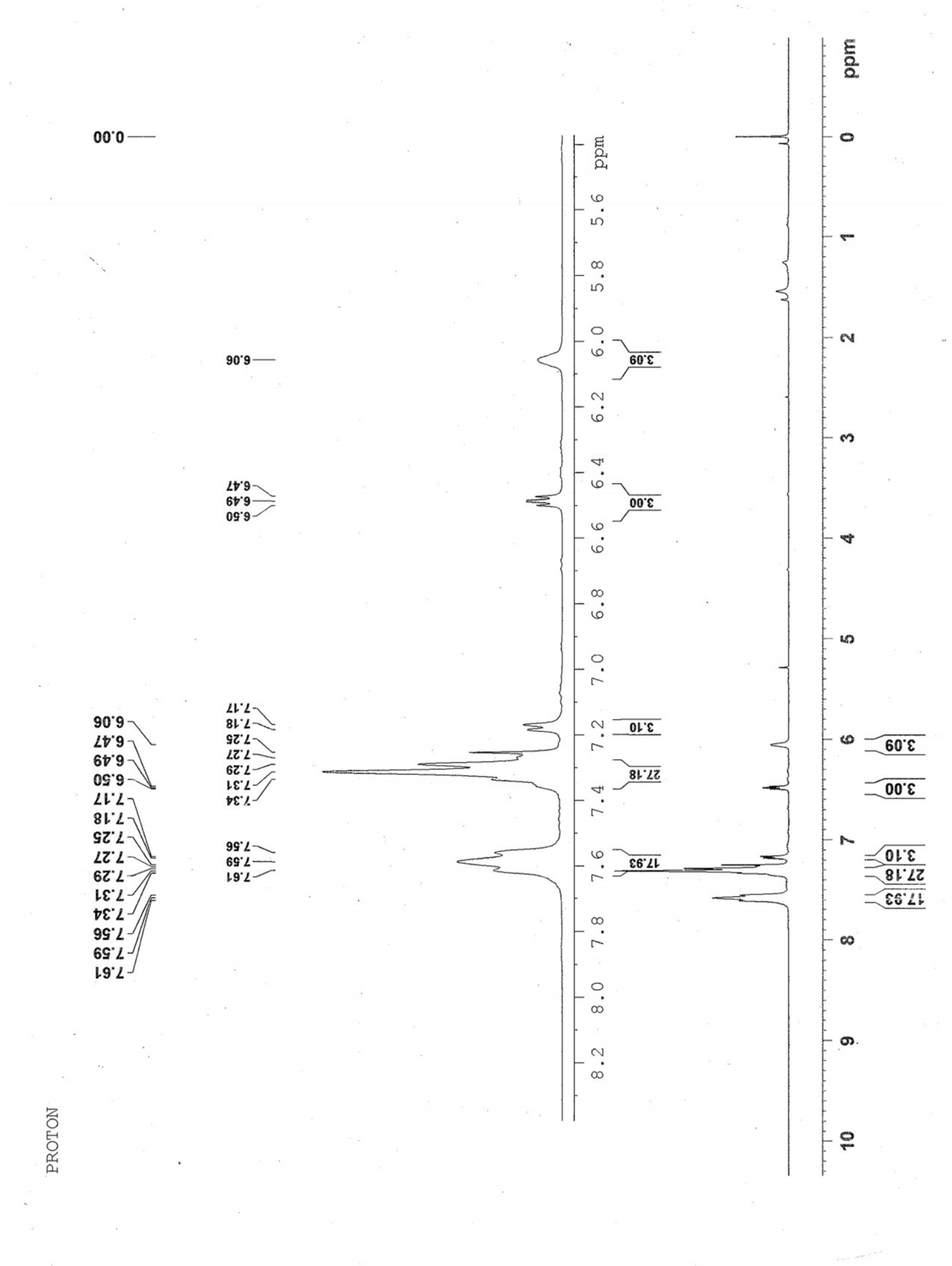
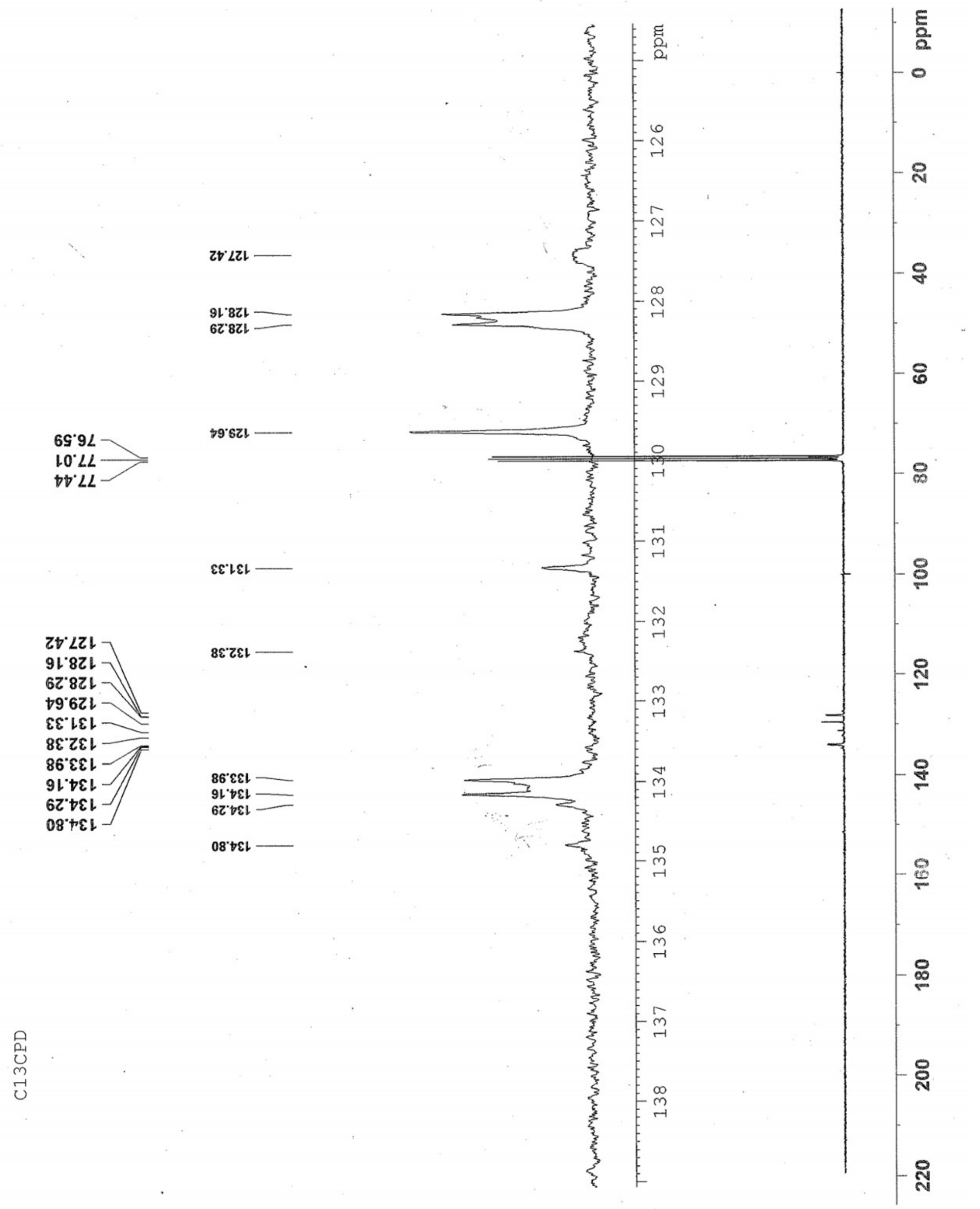


^{31}P NMR of Compound 2c



^{1}H NMR of Compound 2c



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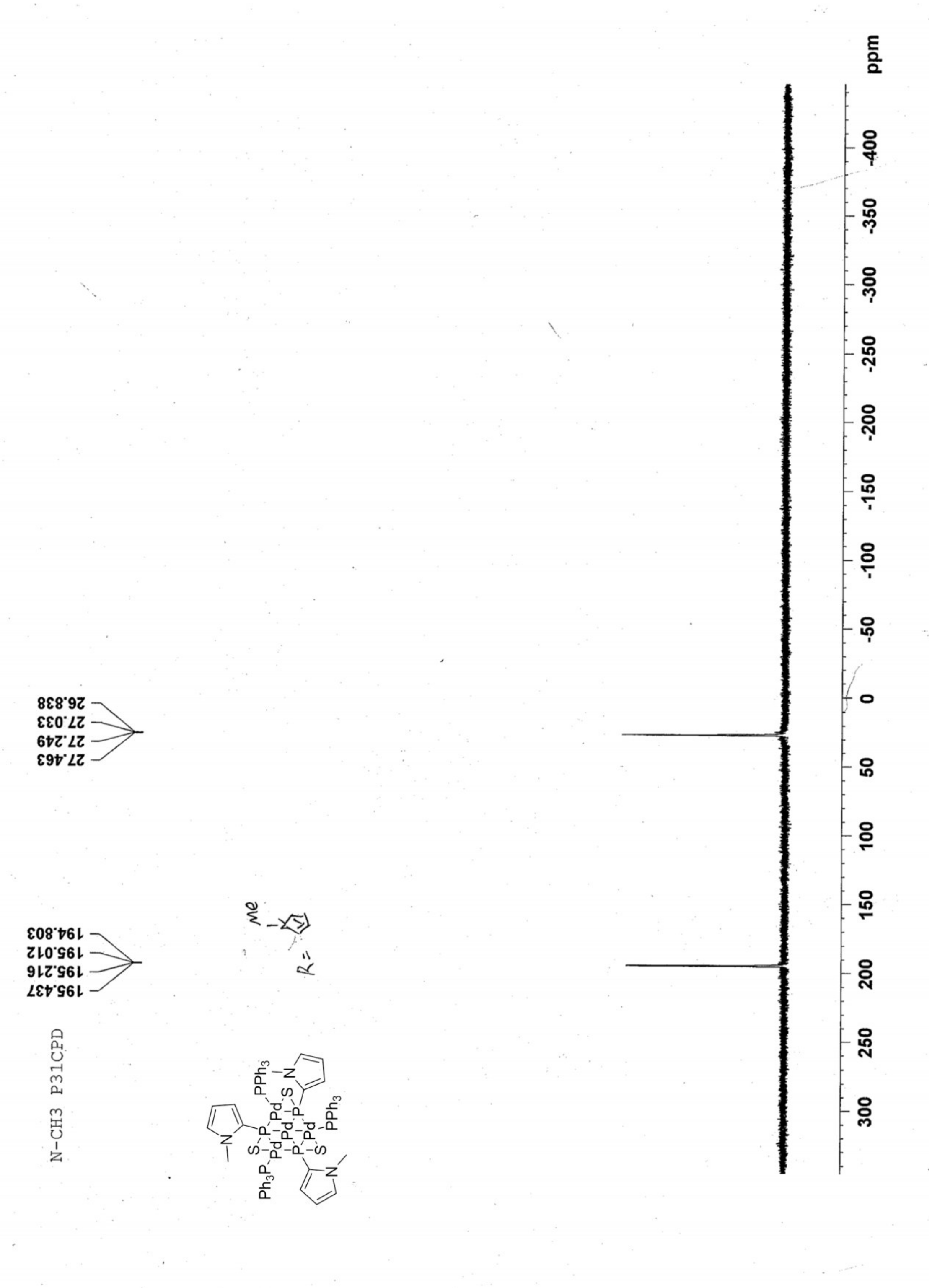
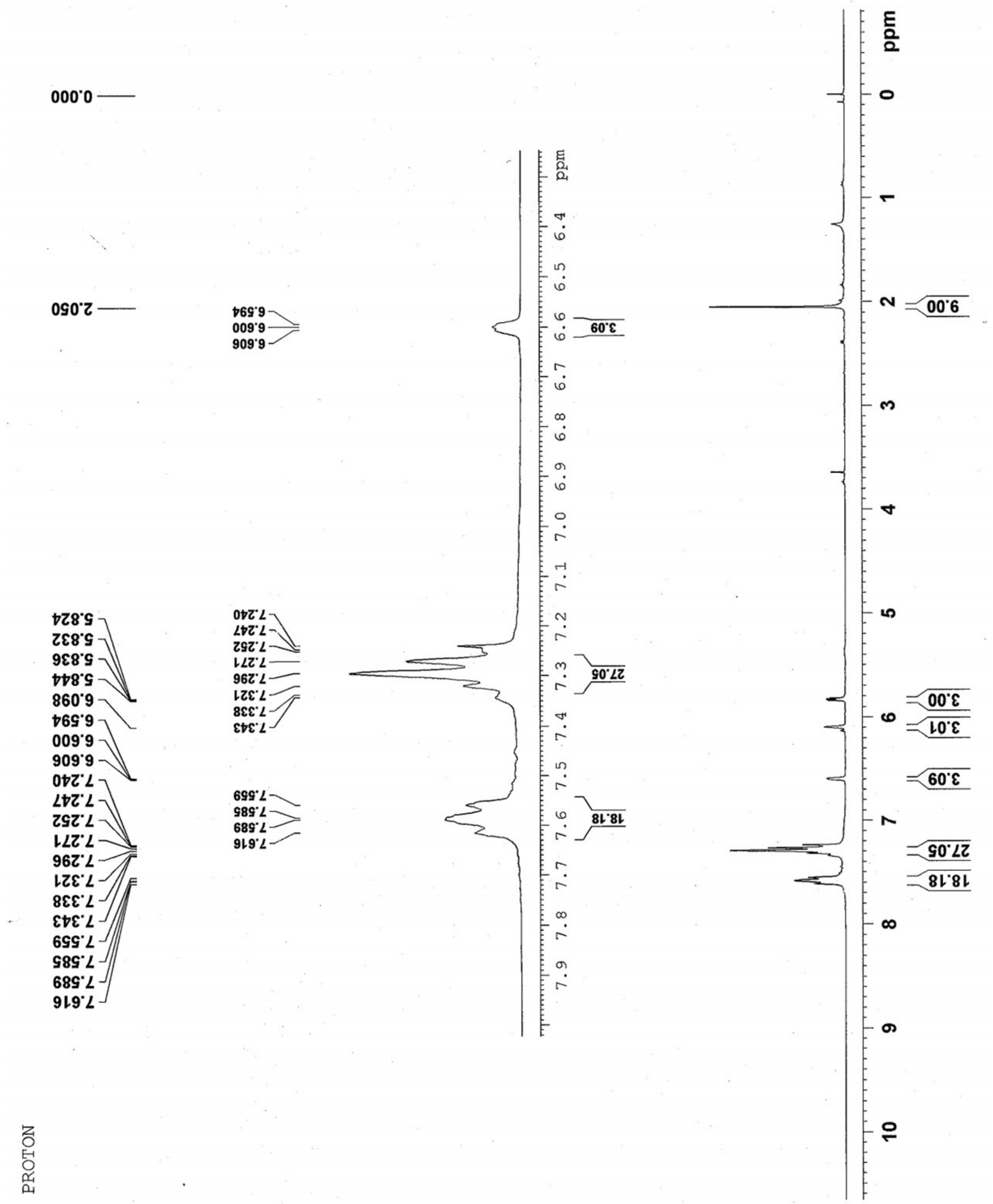


^{31}P NMR of Compound 2d



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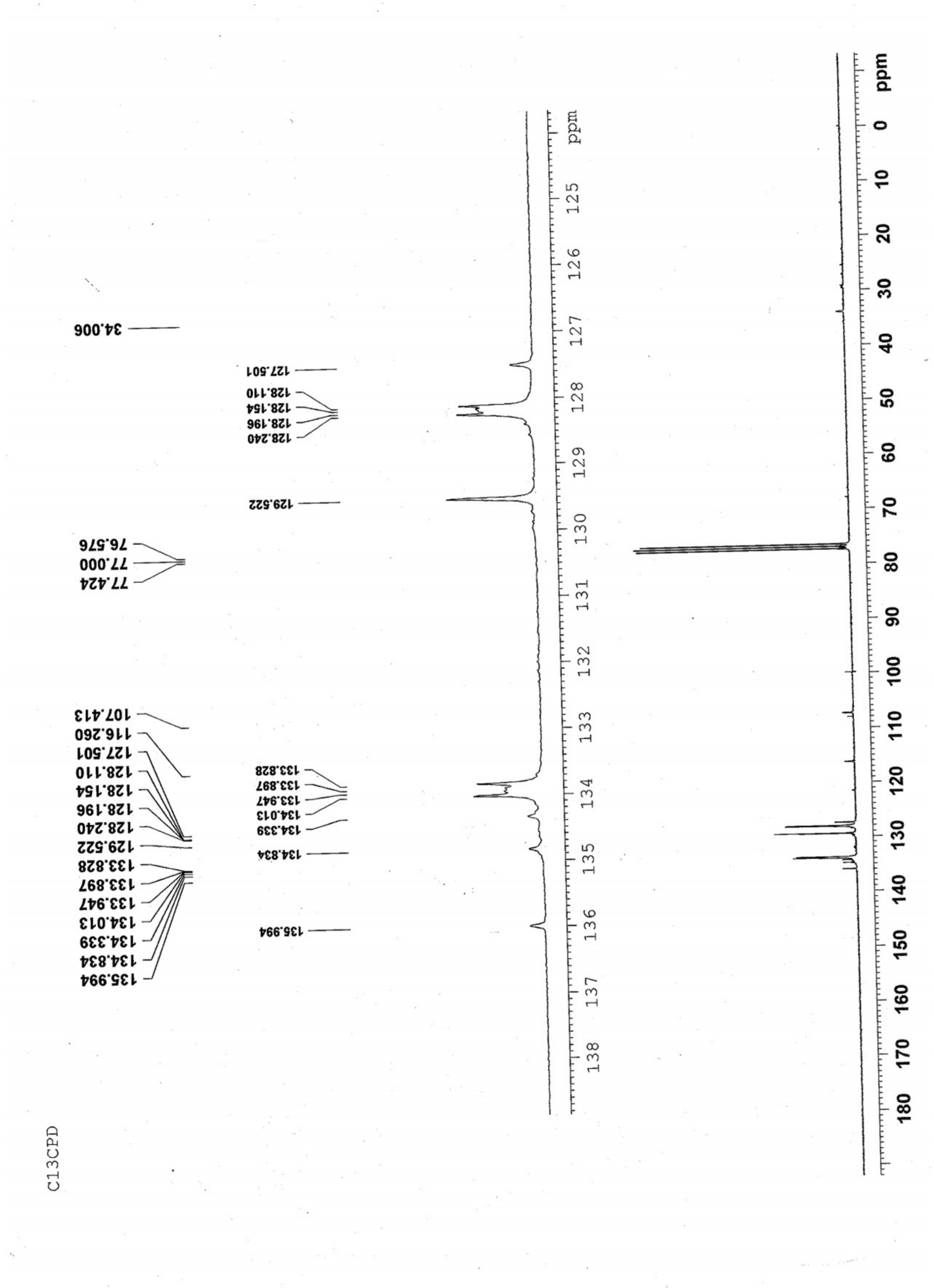
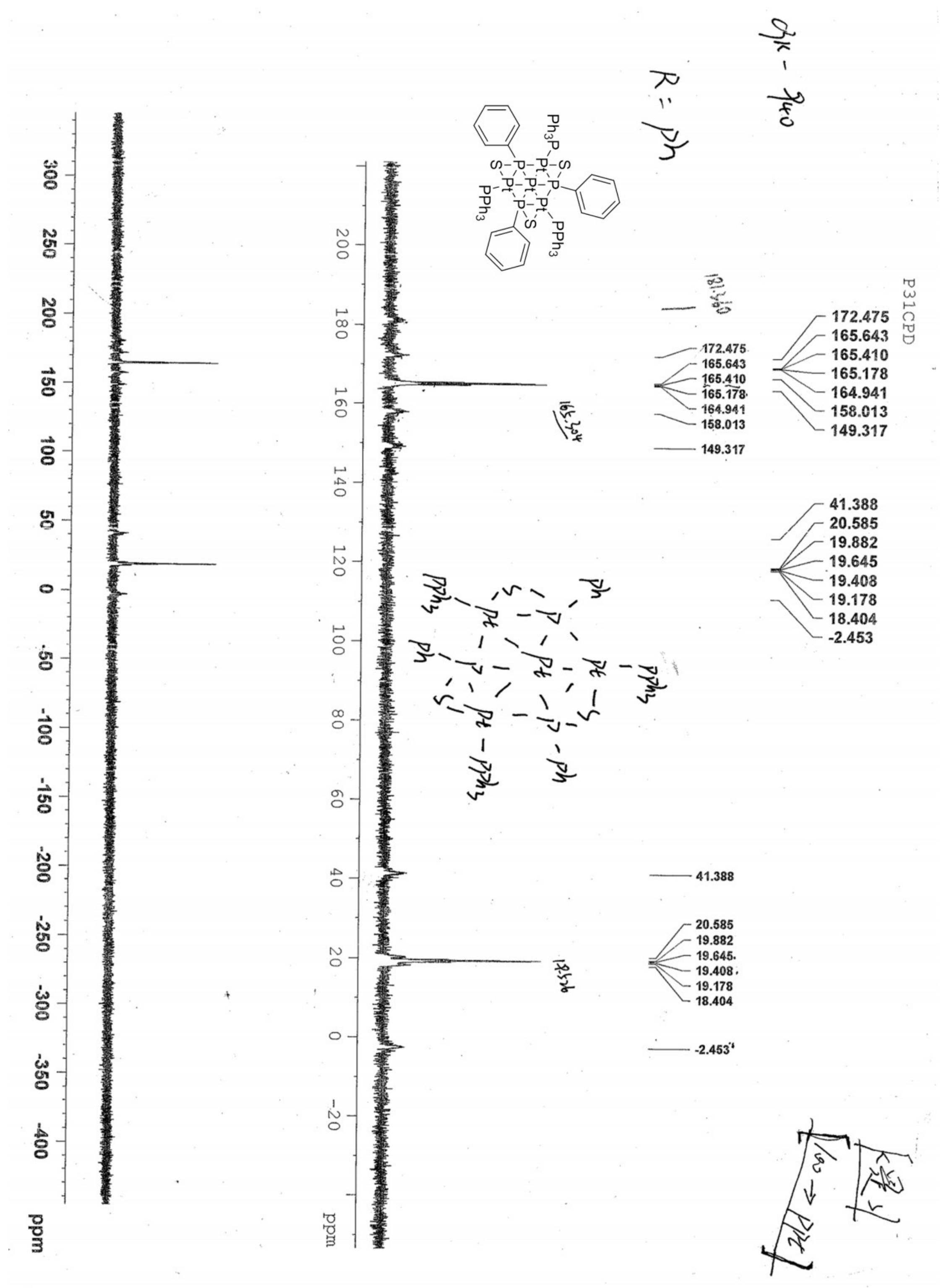
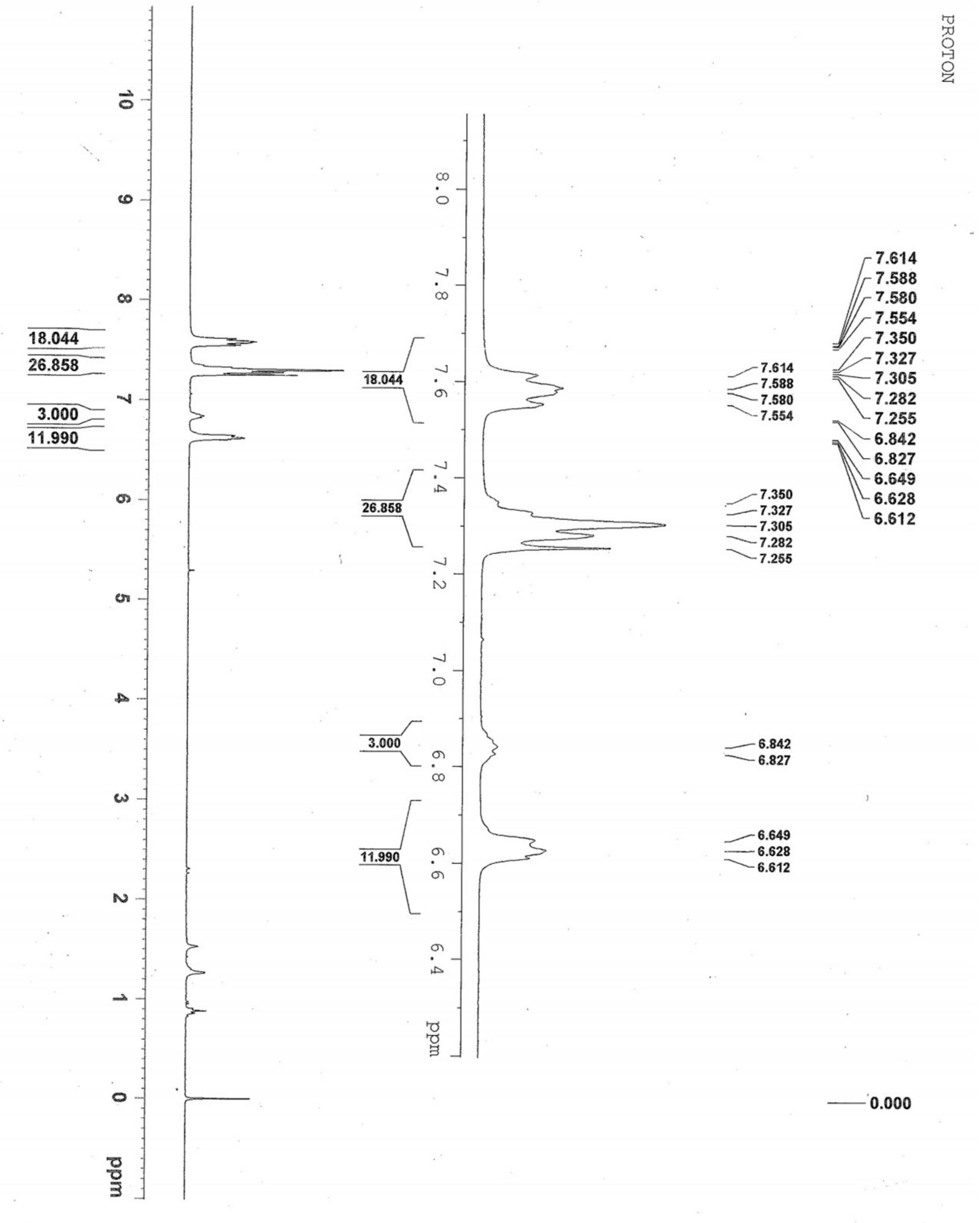


^{13}C NMR of Compound 2d



^{31}P NMR of Compound 4a



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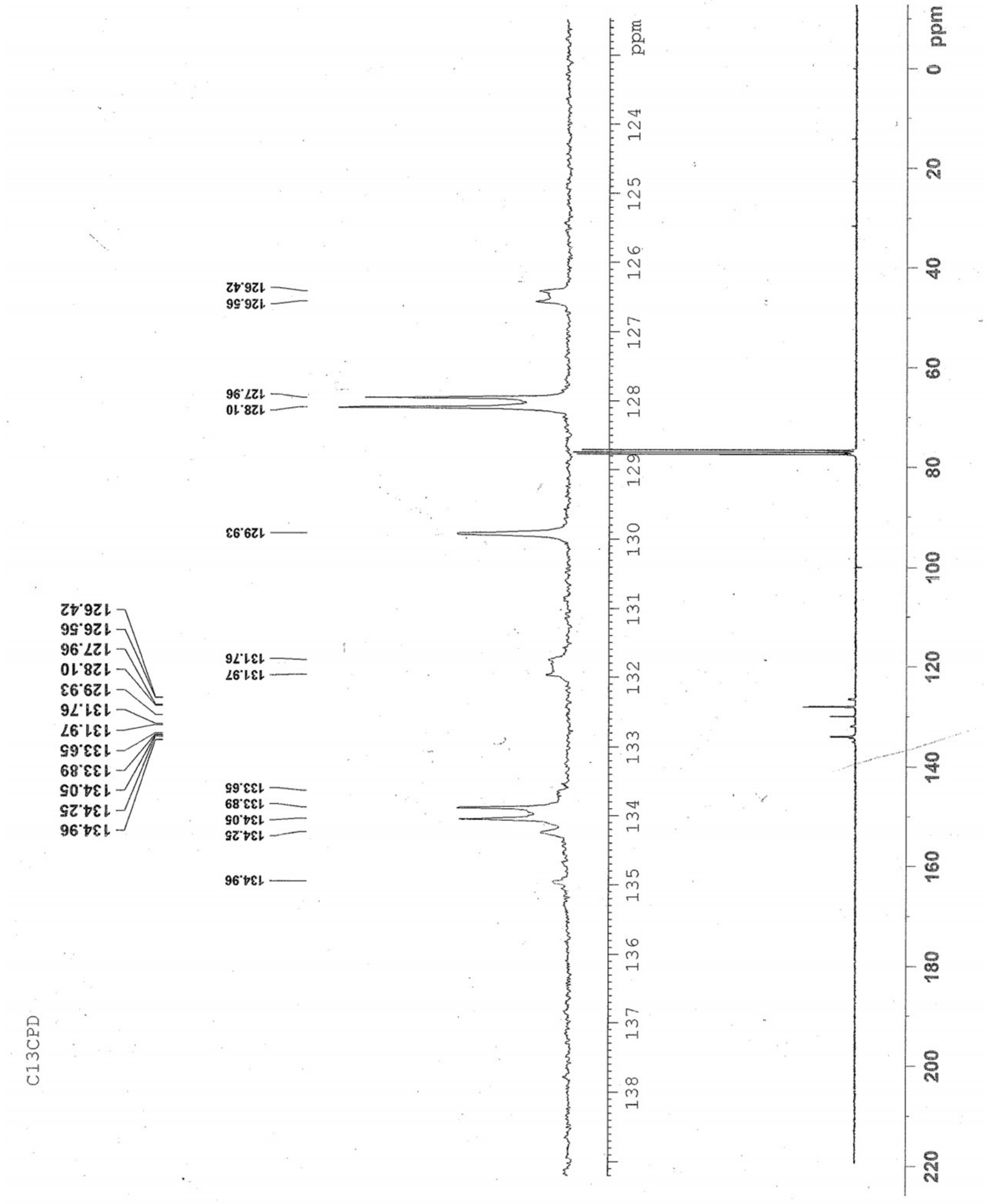

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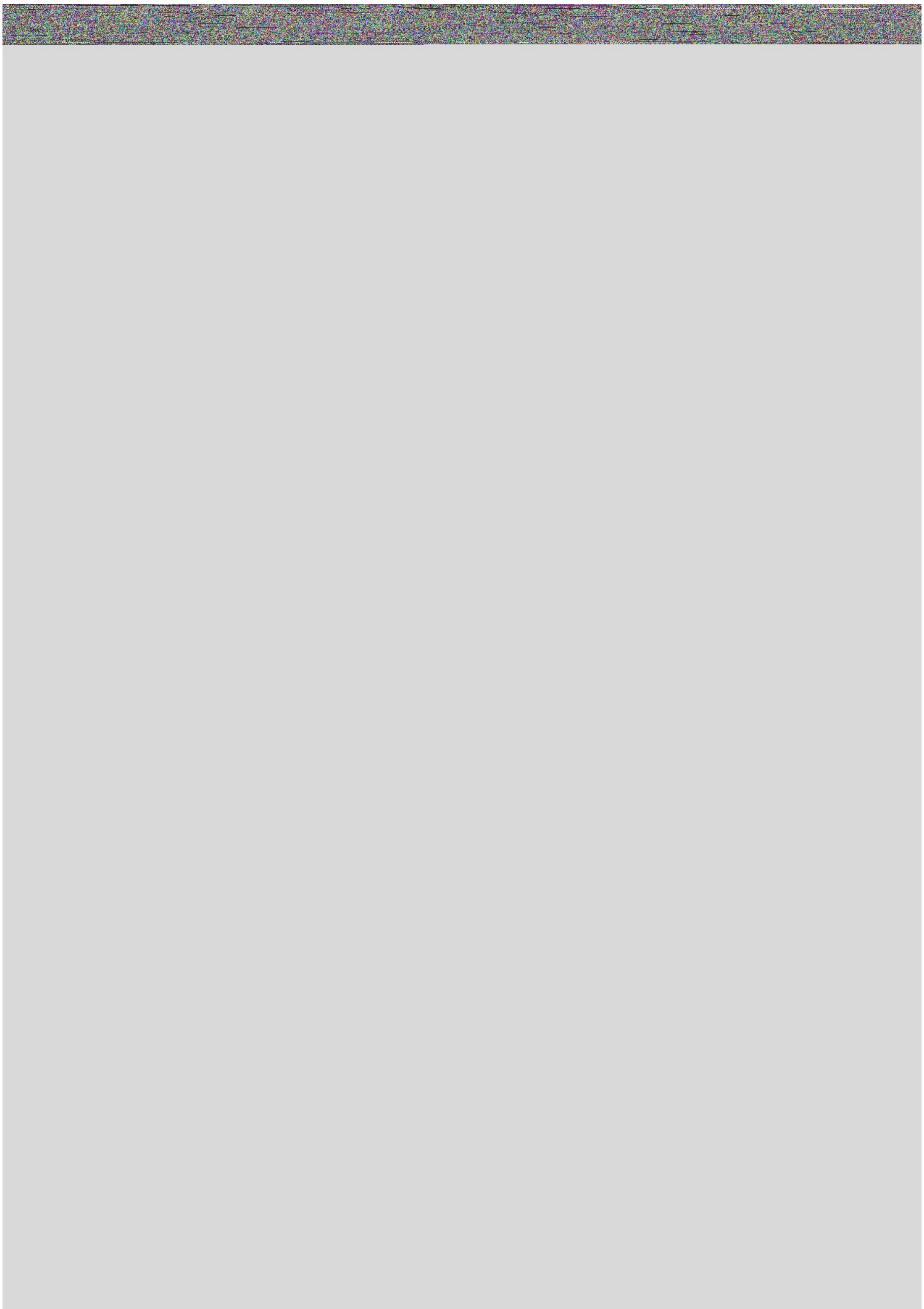
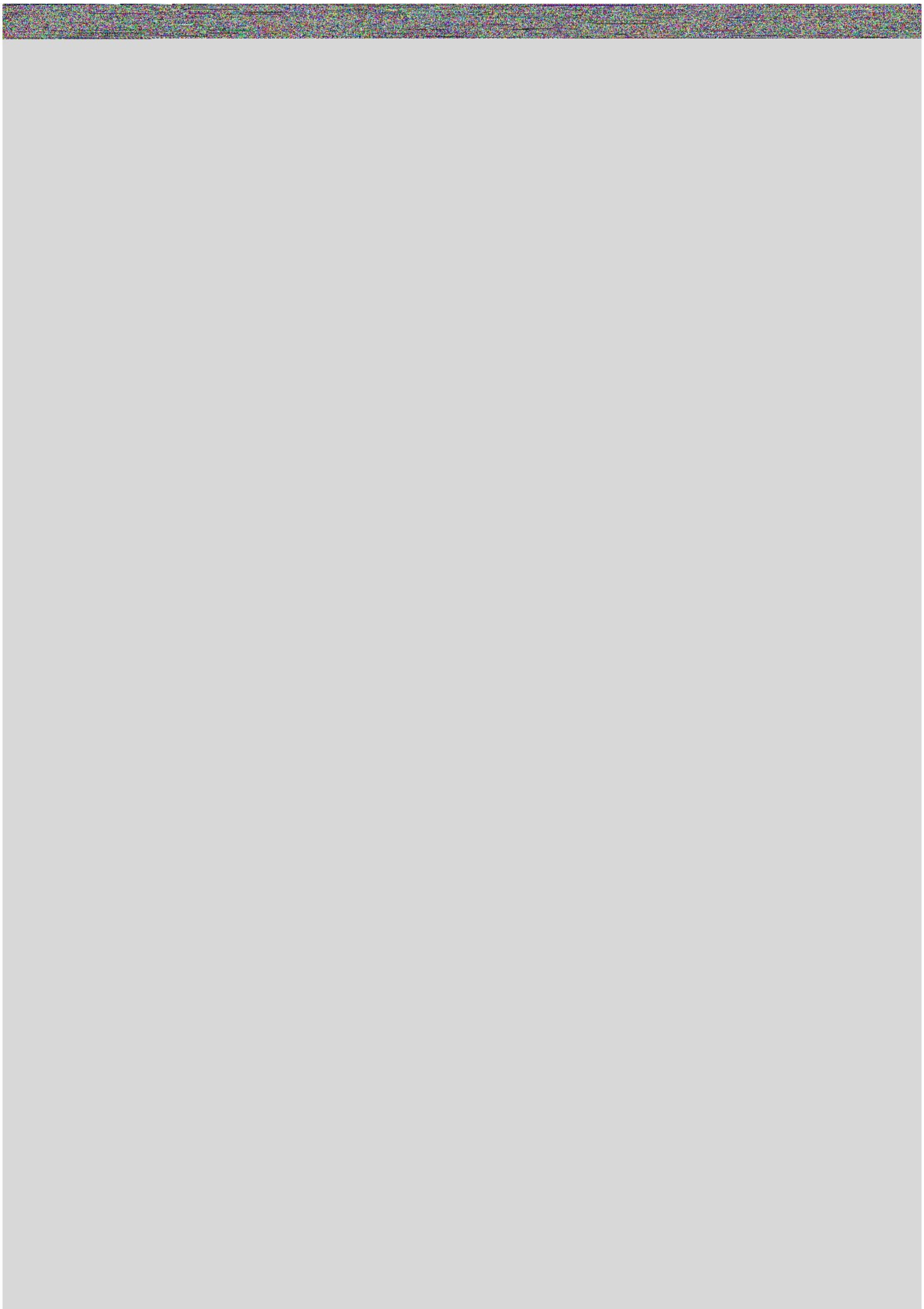


^{1}H NMR of Compound 1c



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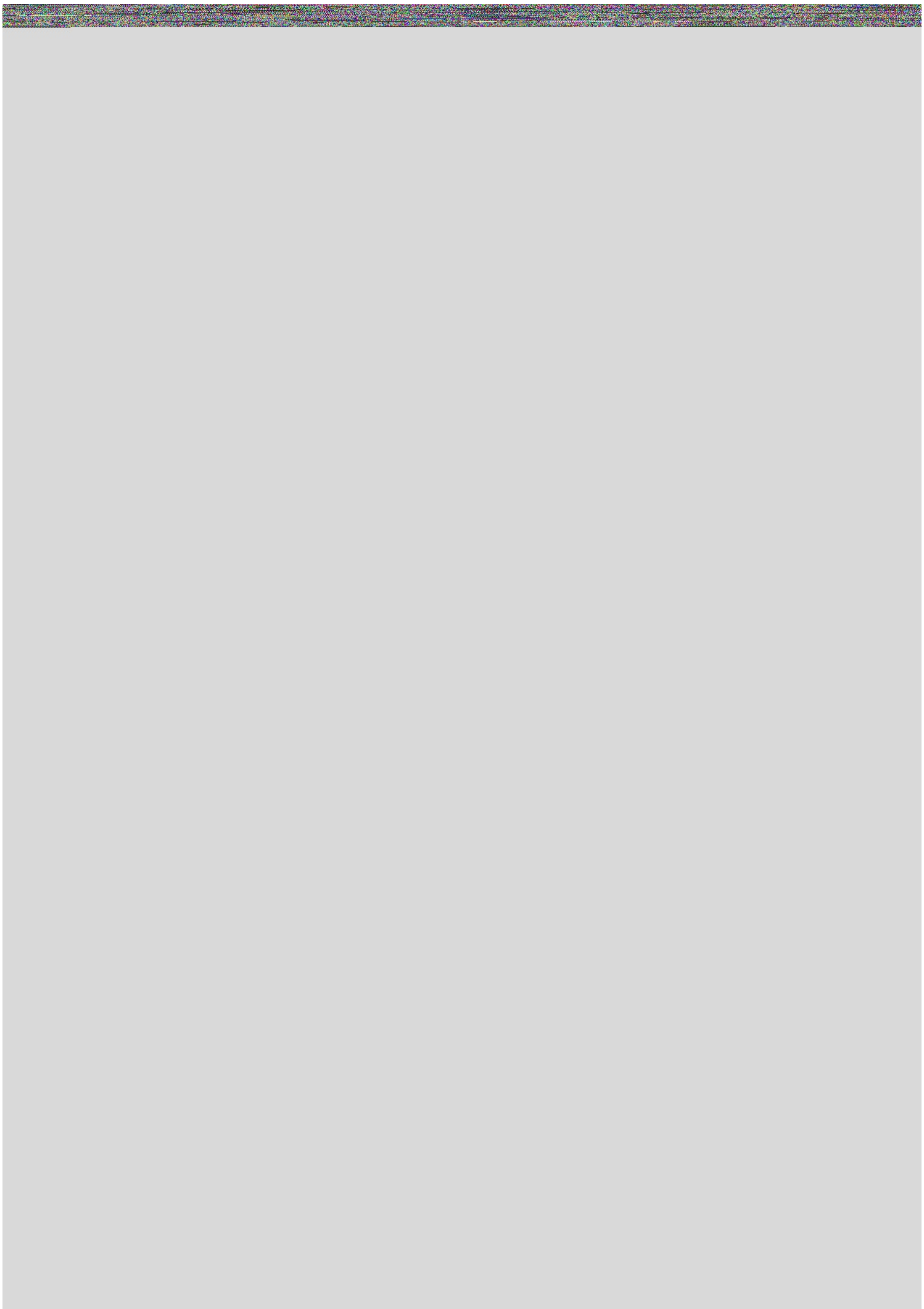

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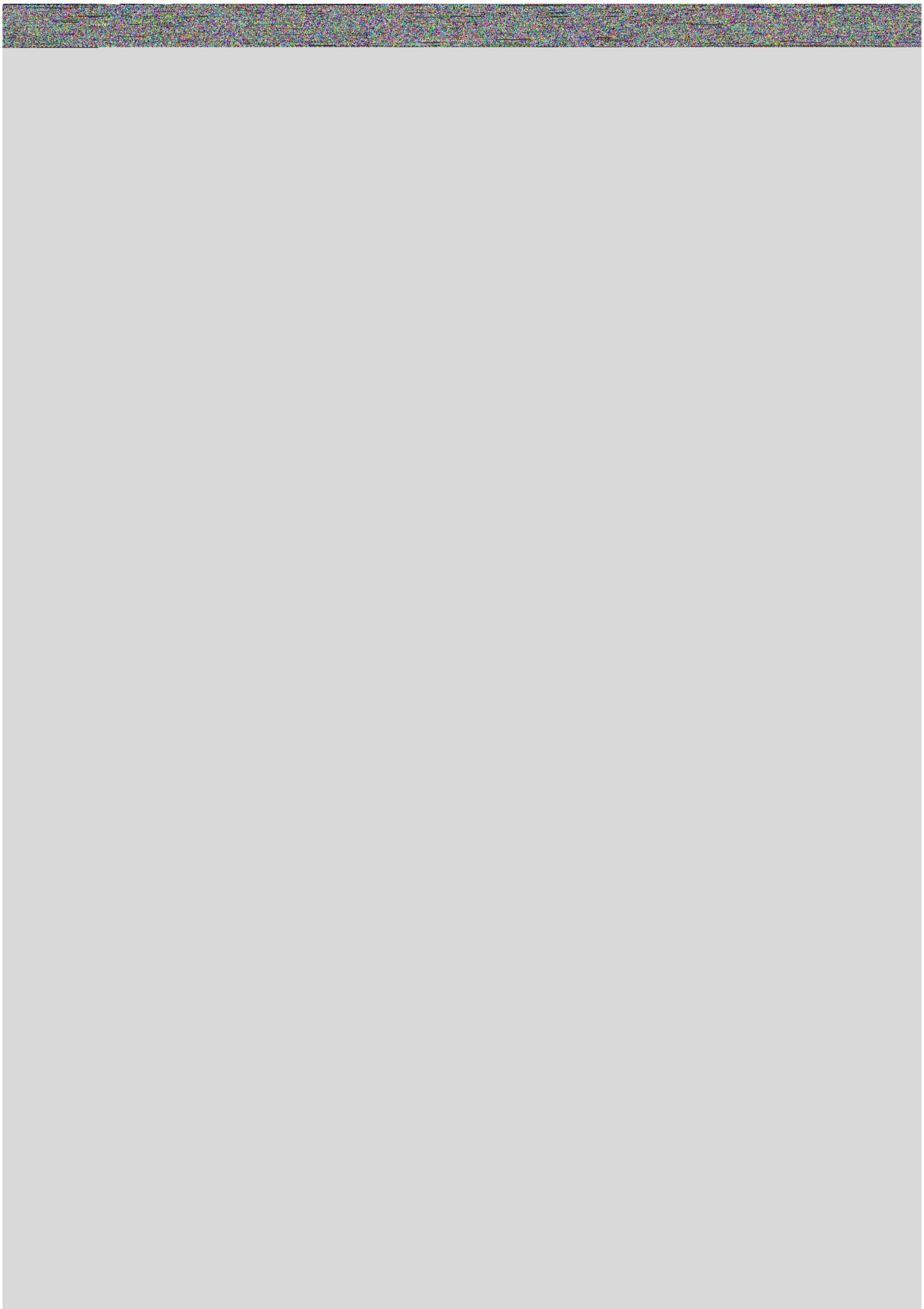

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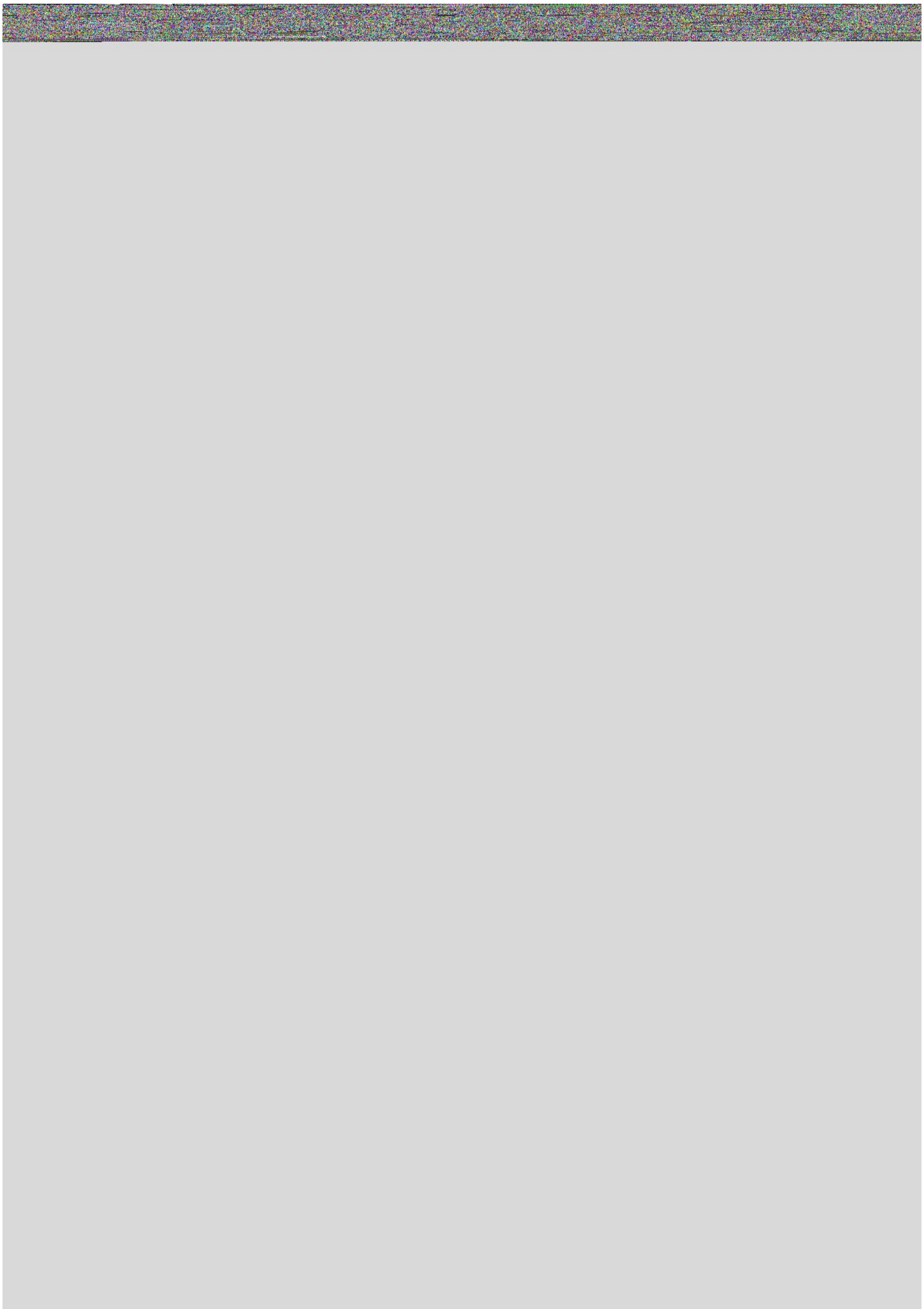

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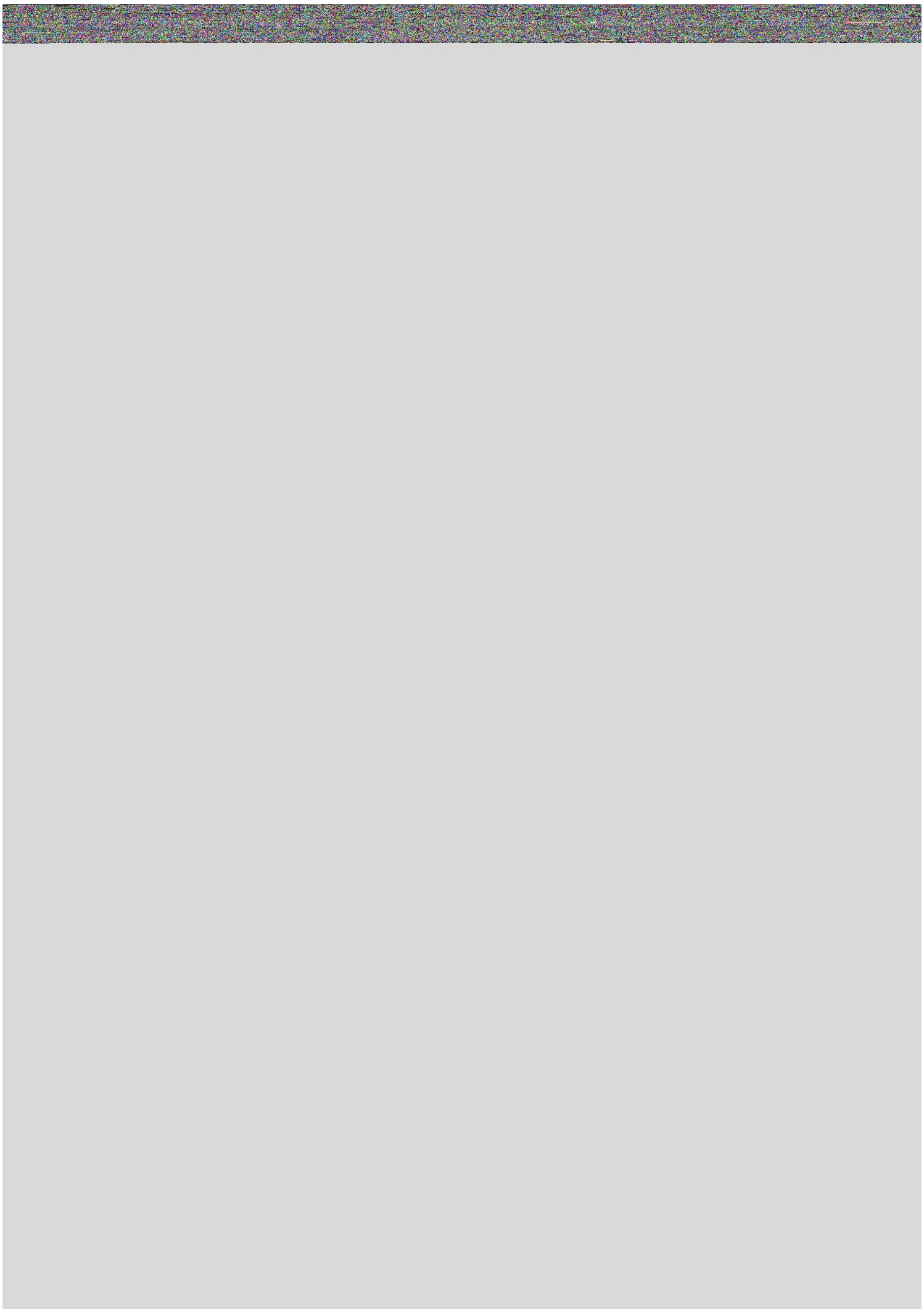
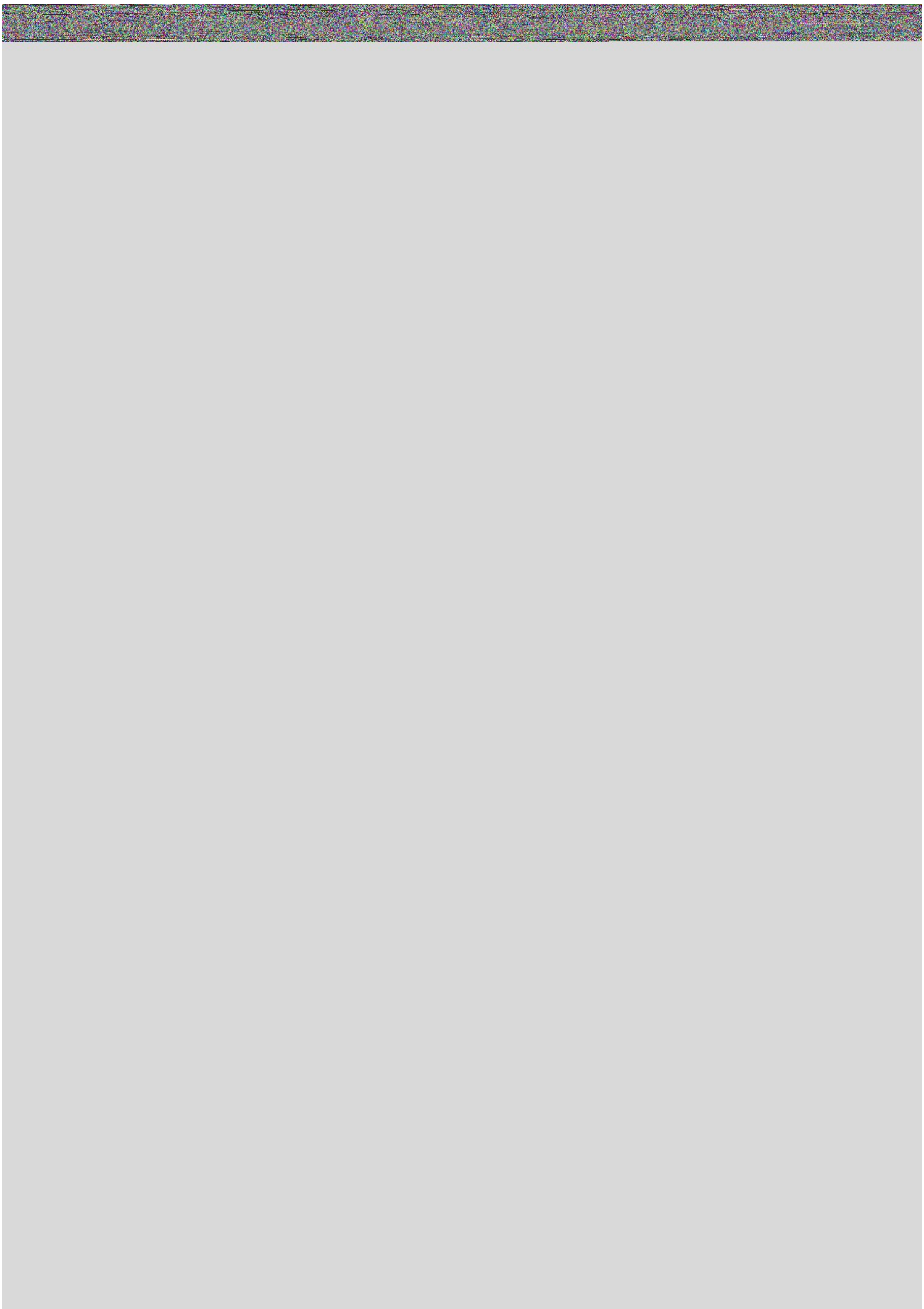


^{31}P NMR of Compound 2a



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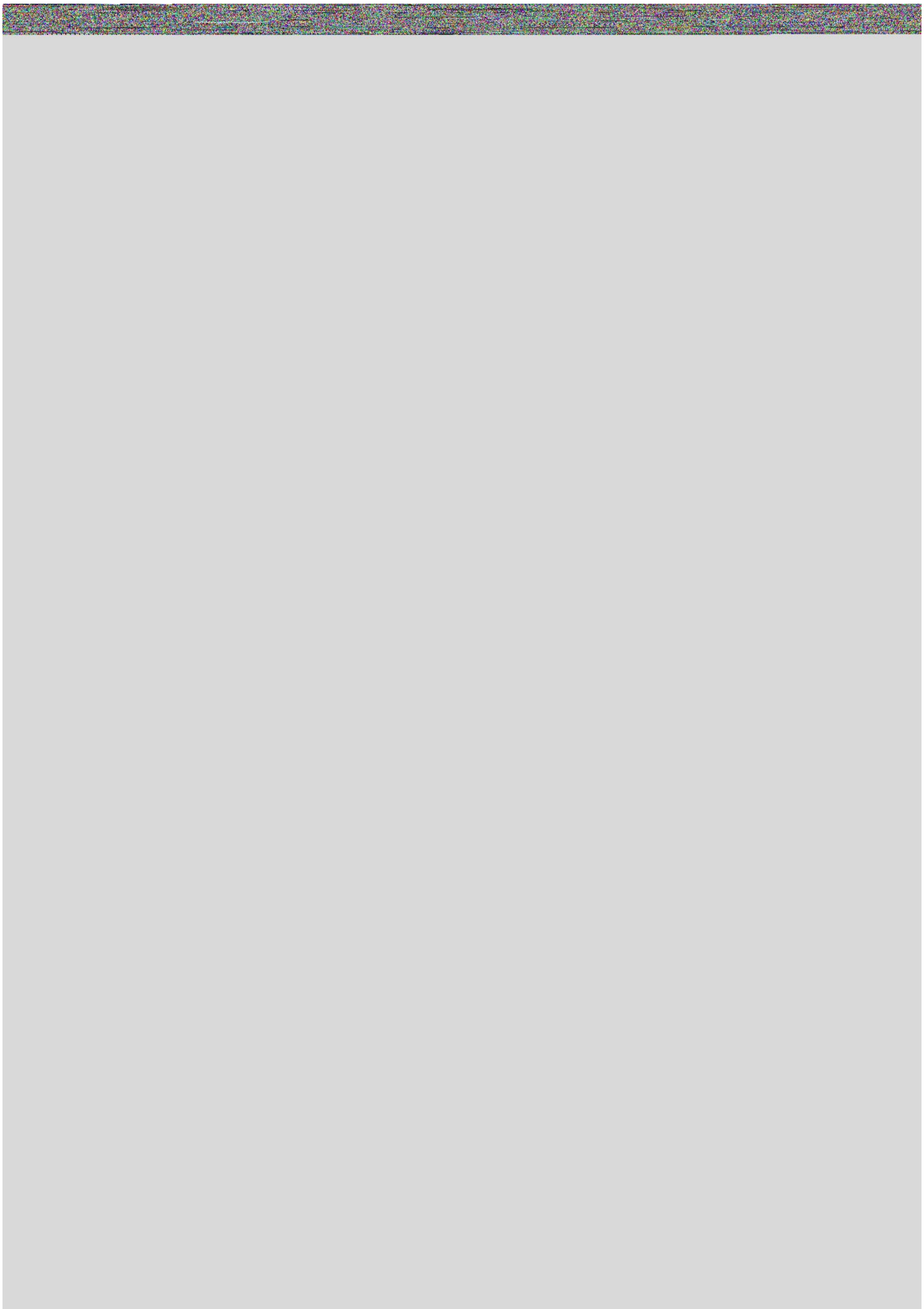

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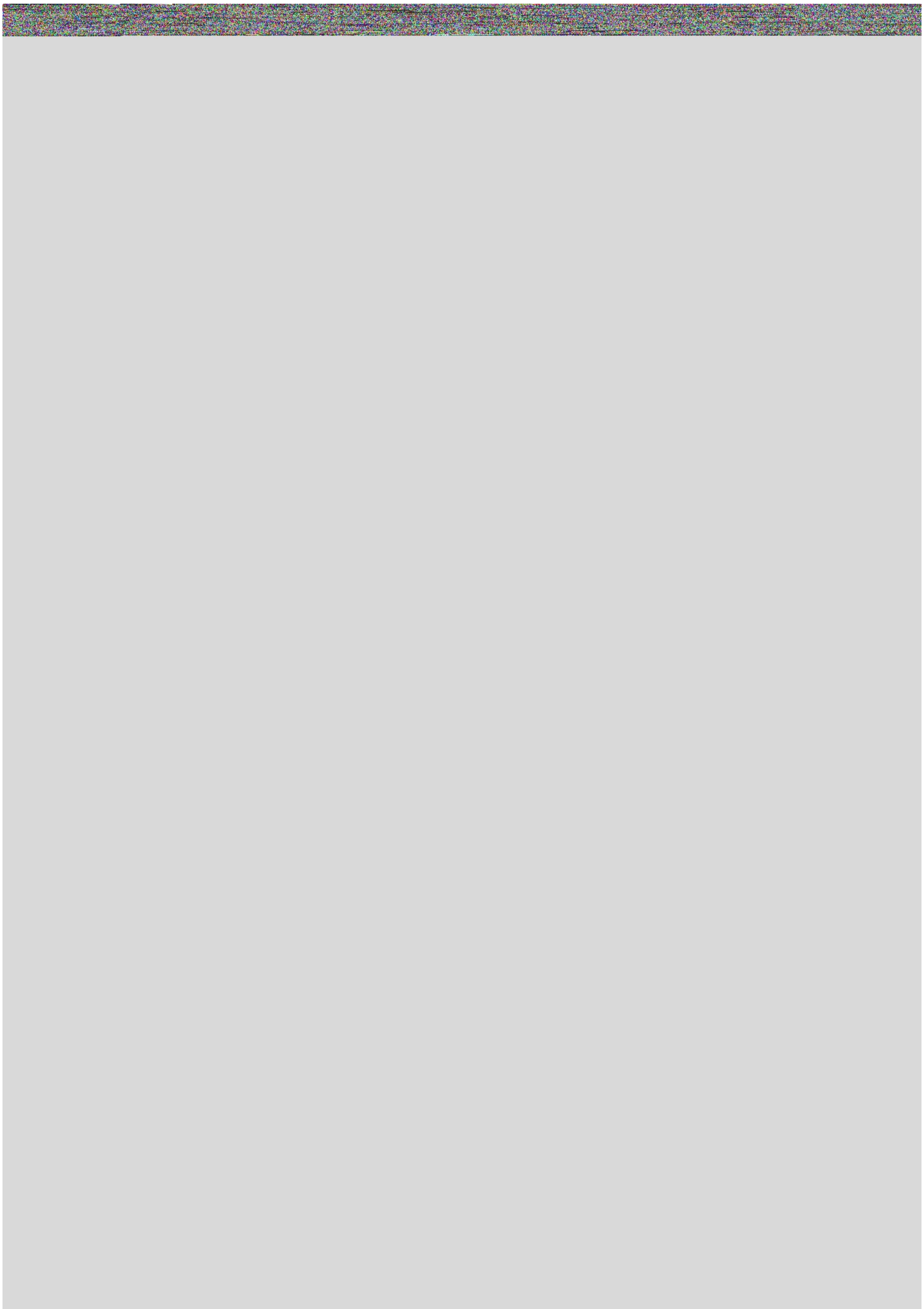

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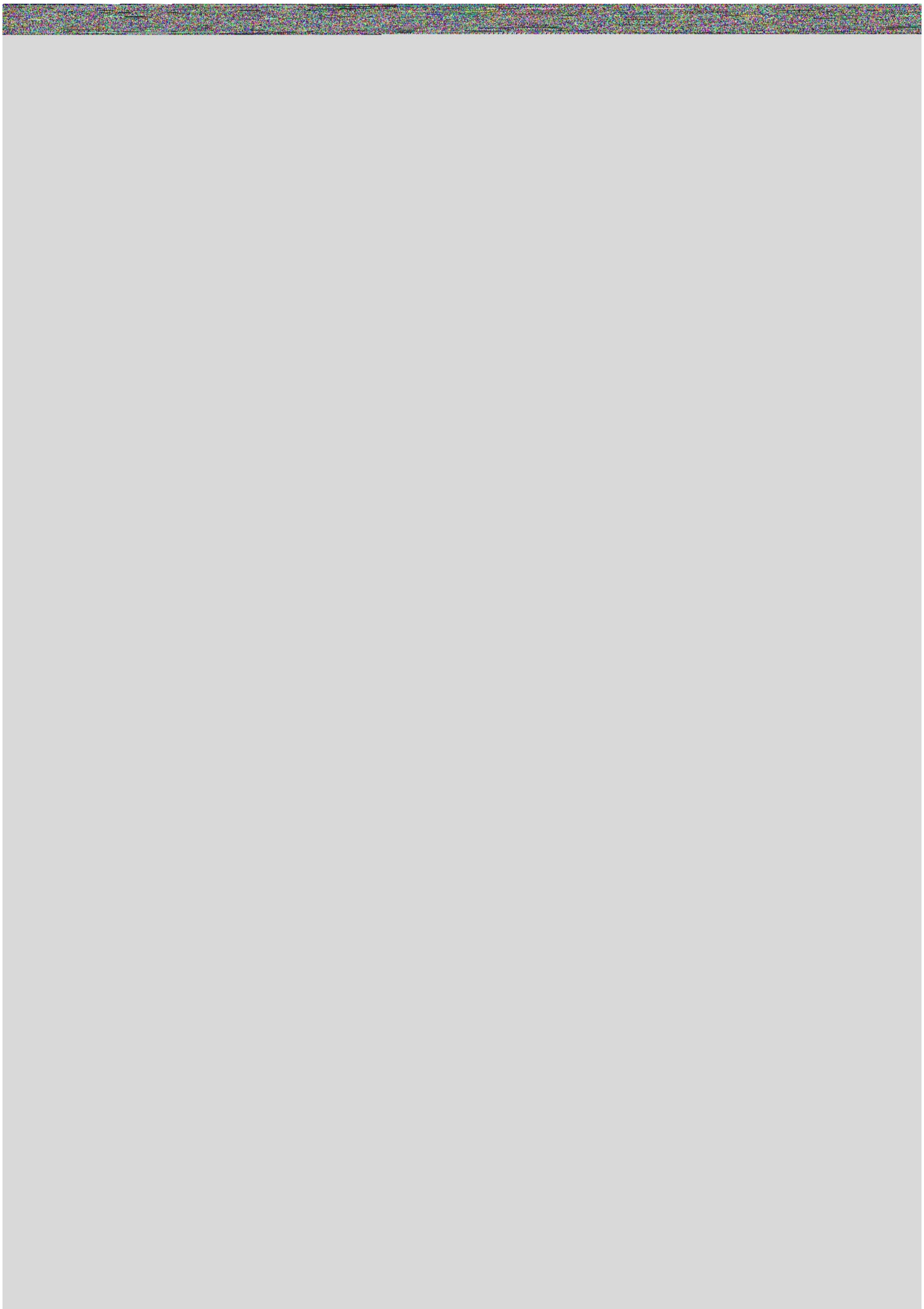

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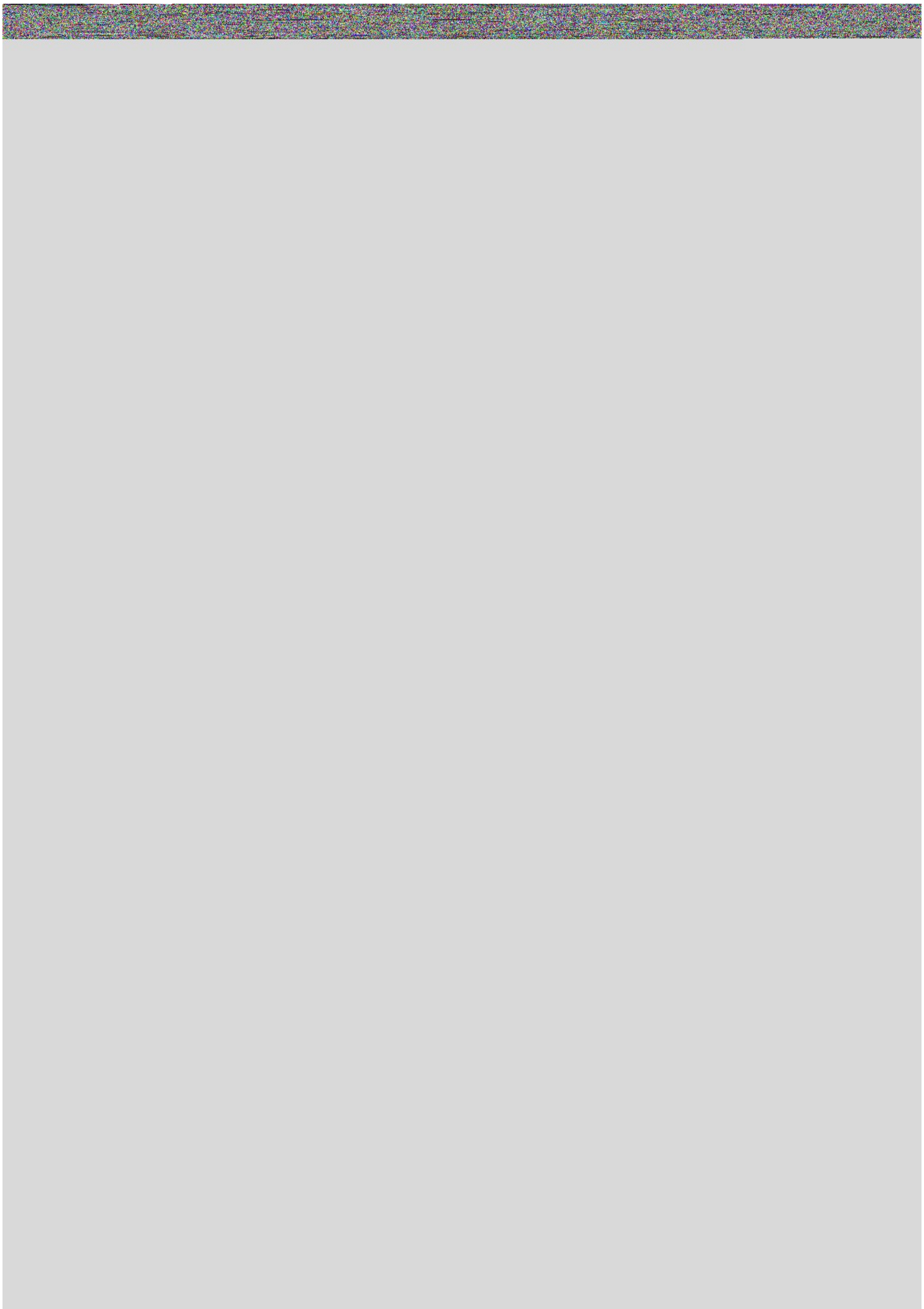

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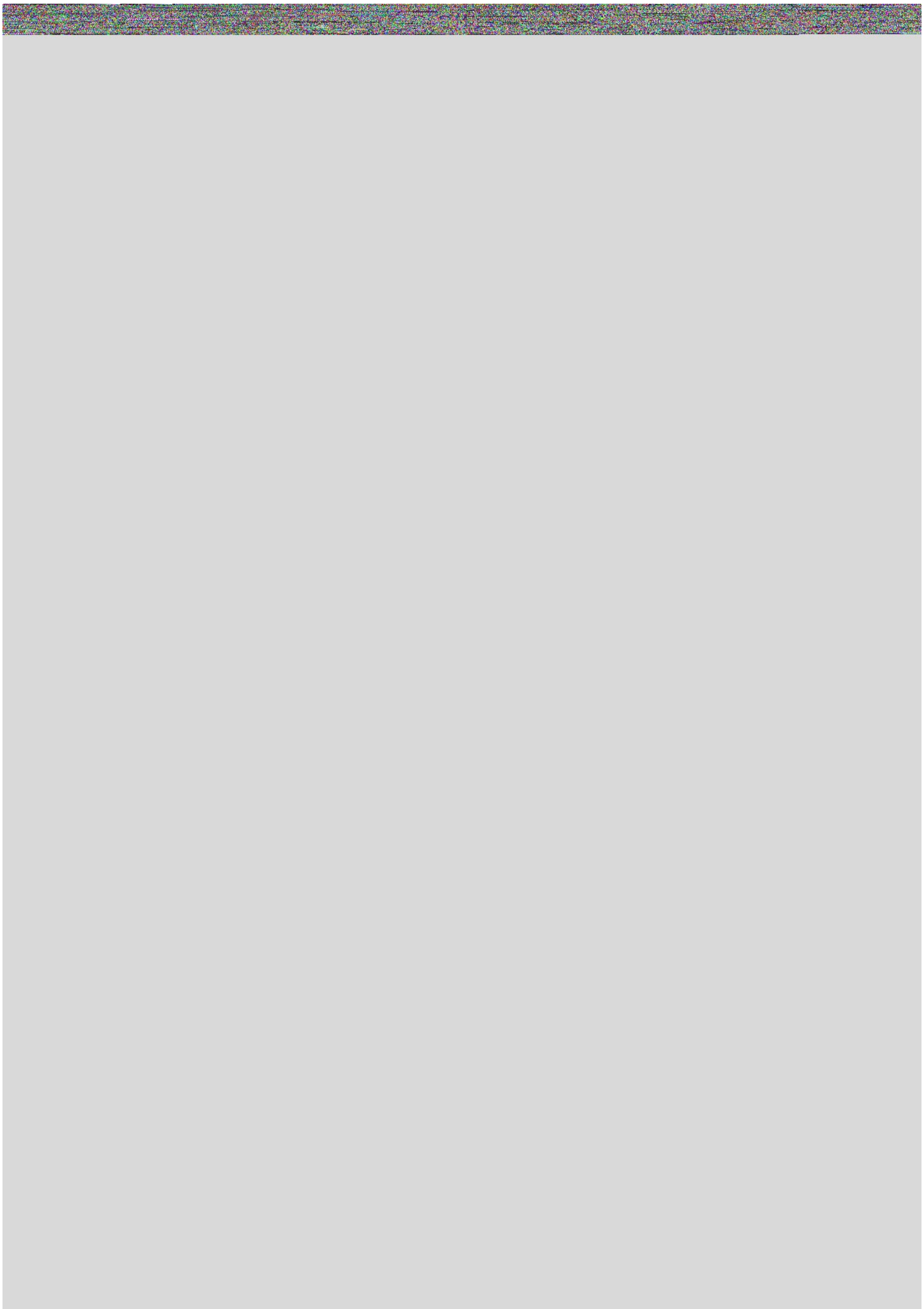

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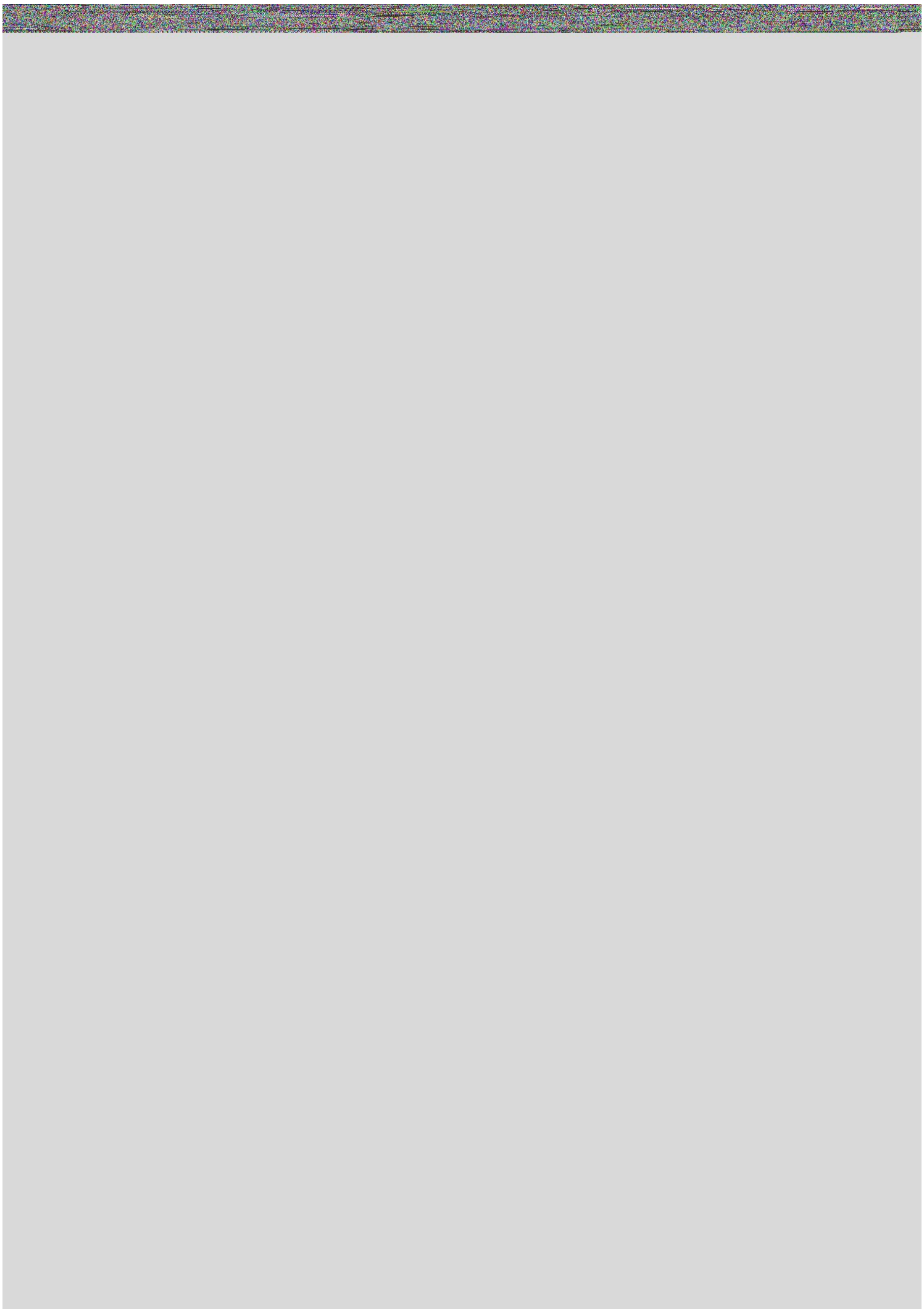

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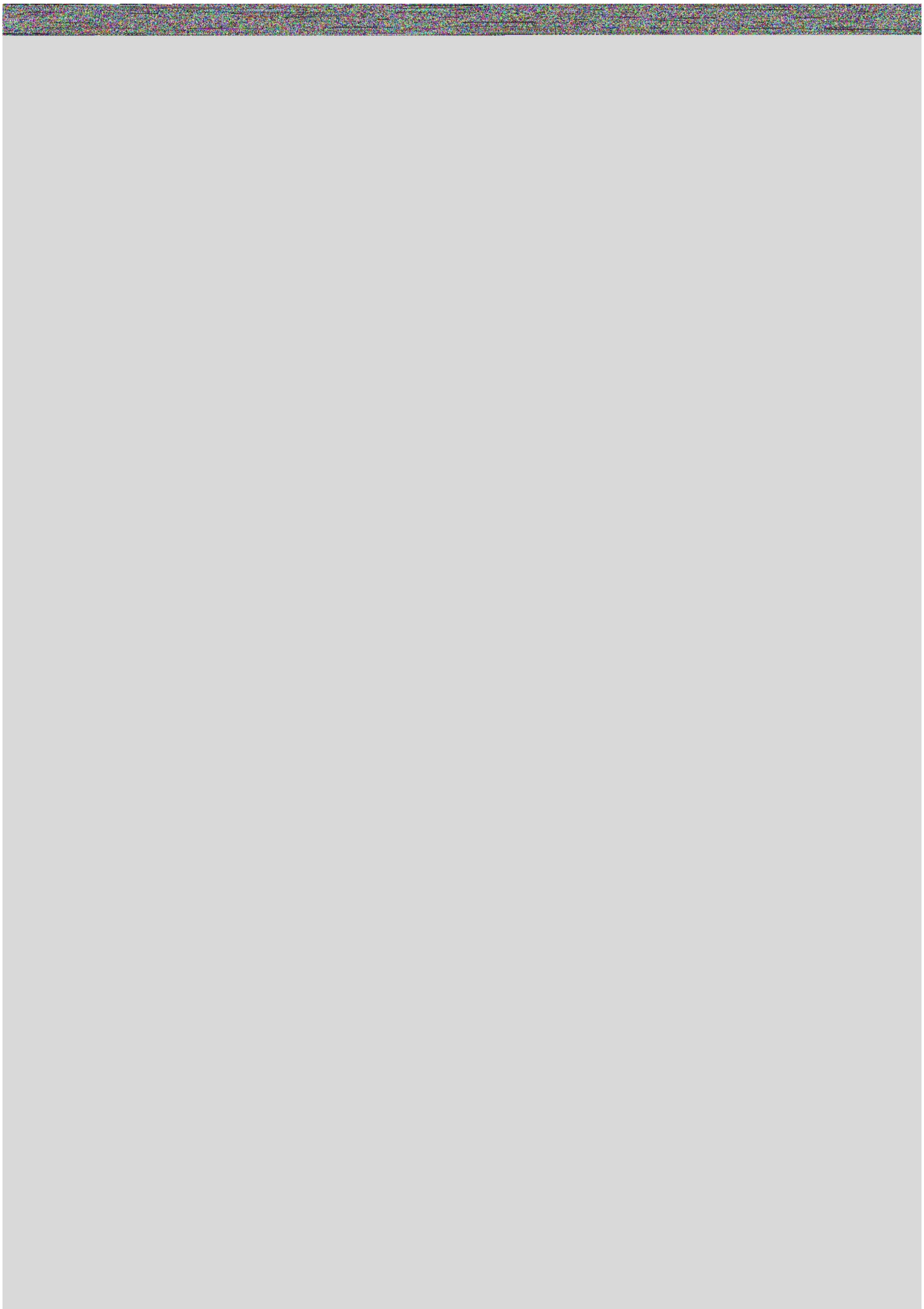

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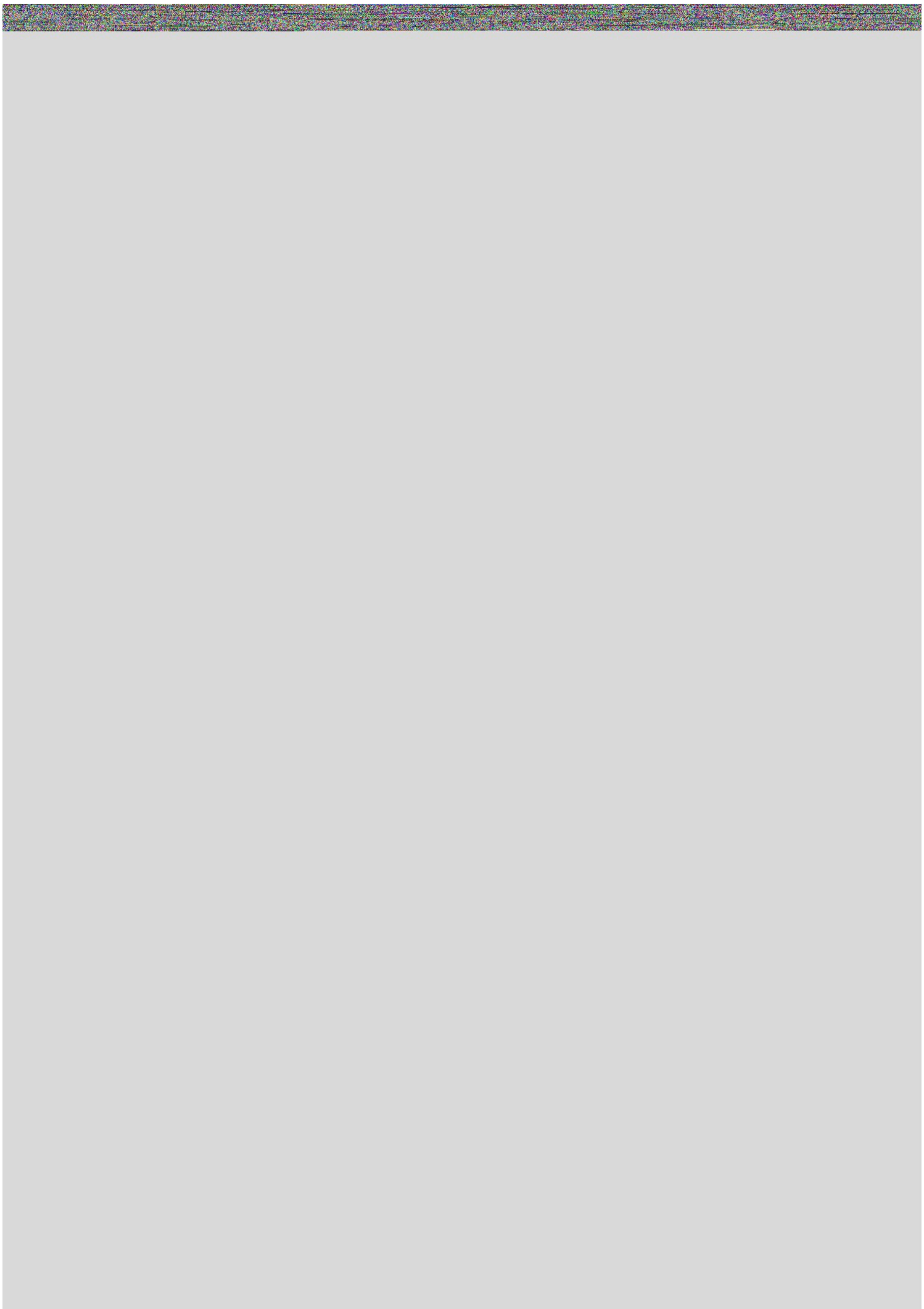
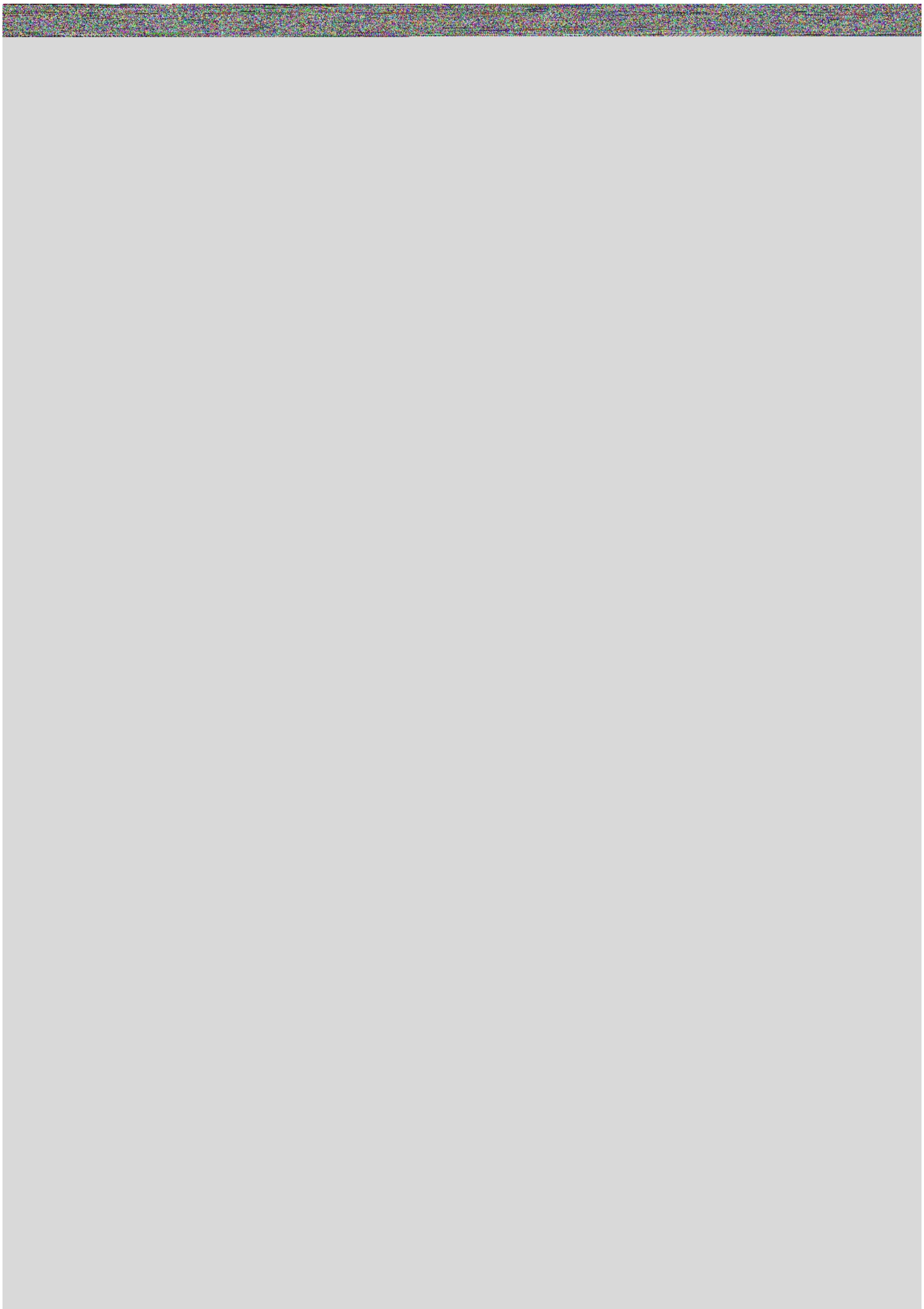


^{31}P NMR of Compound 2d



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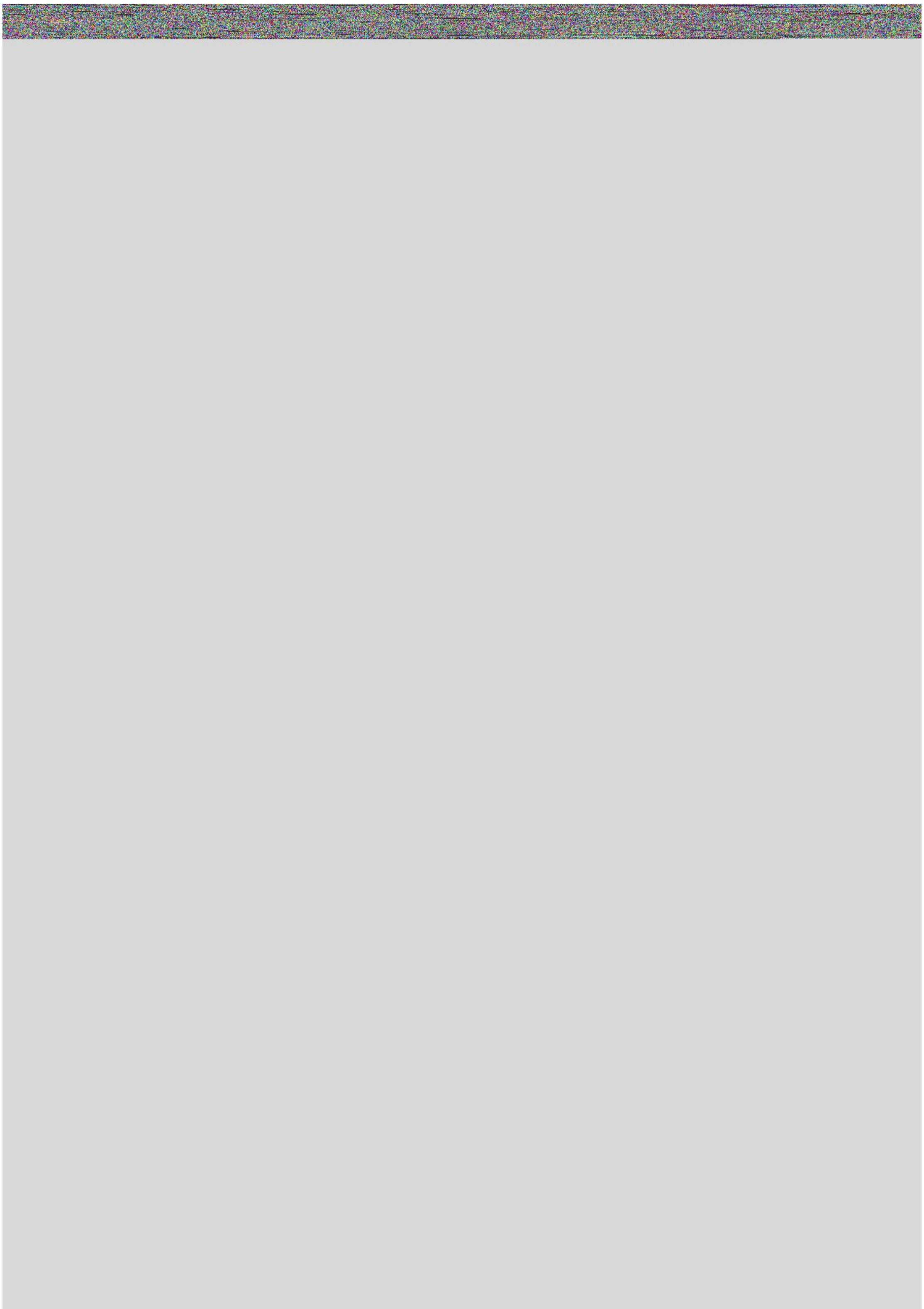

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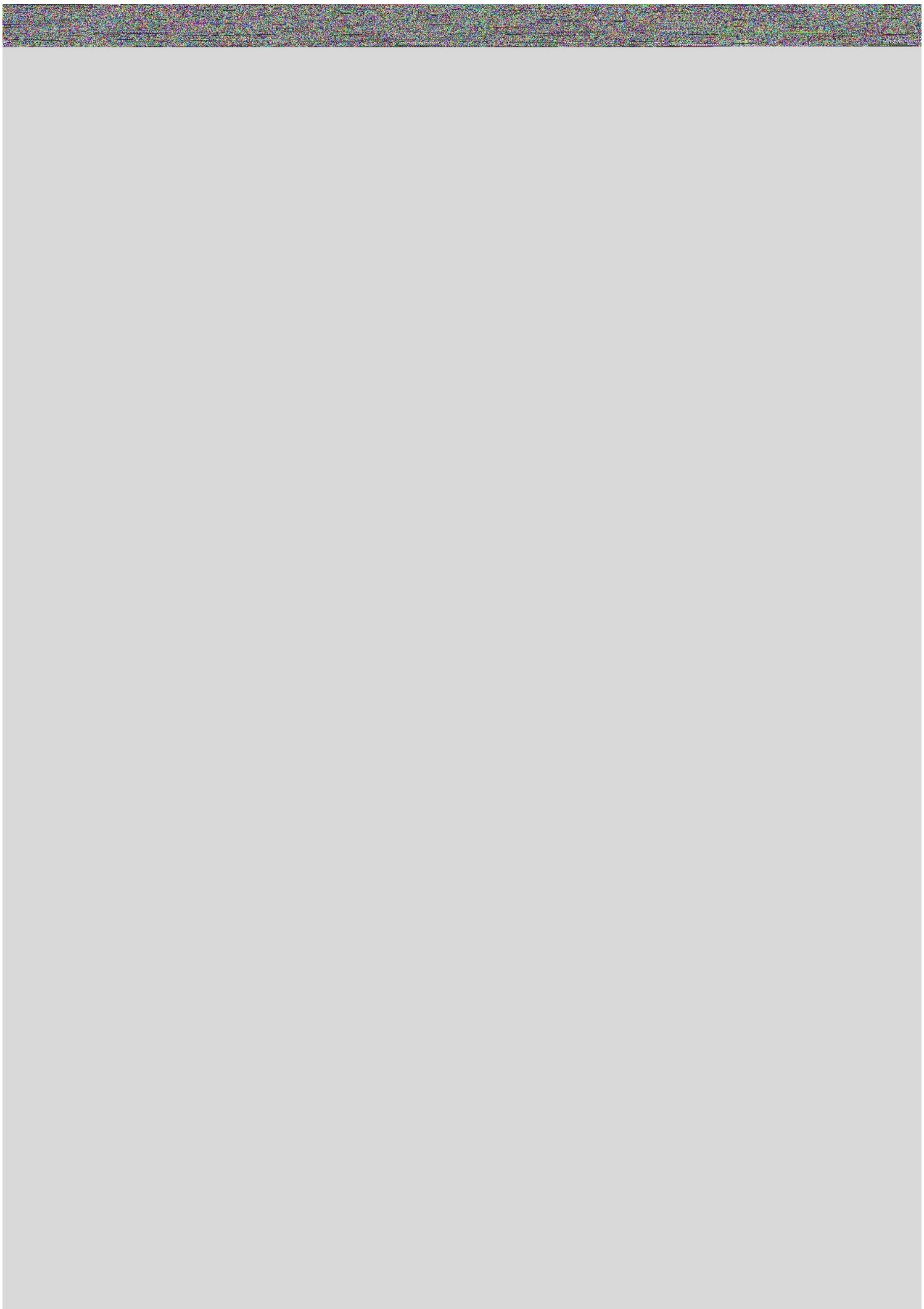
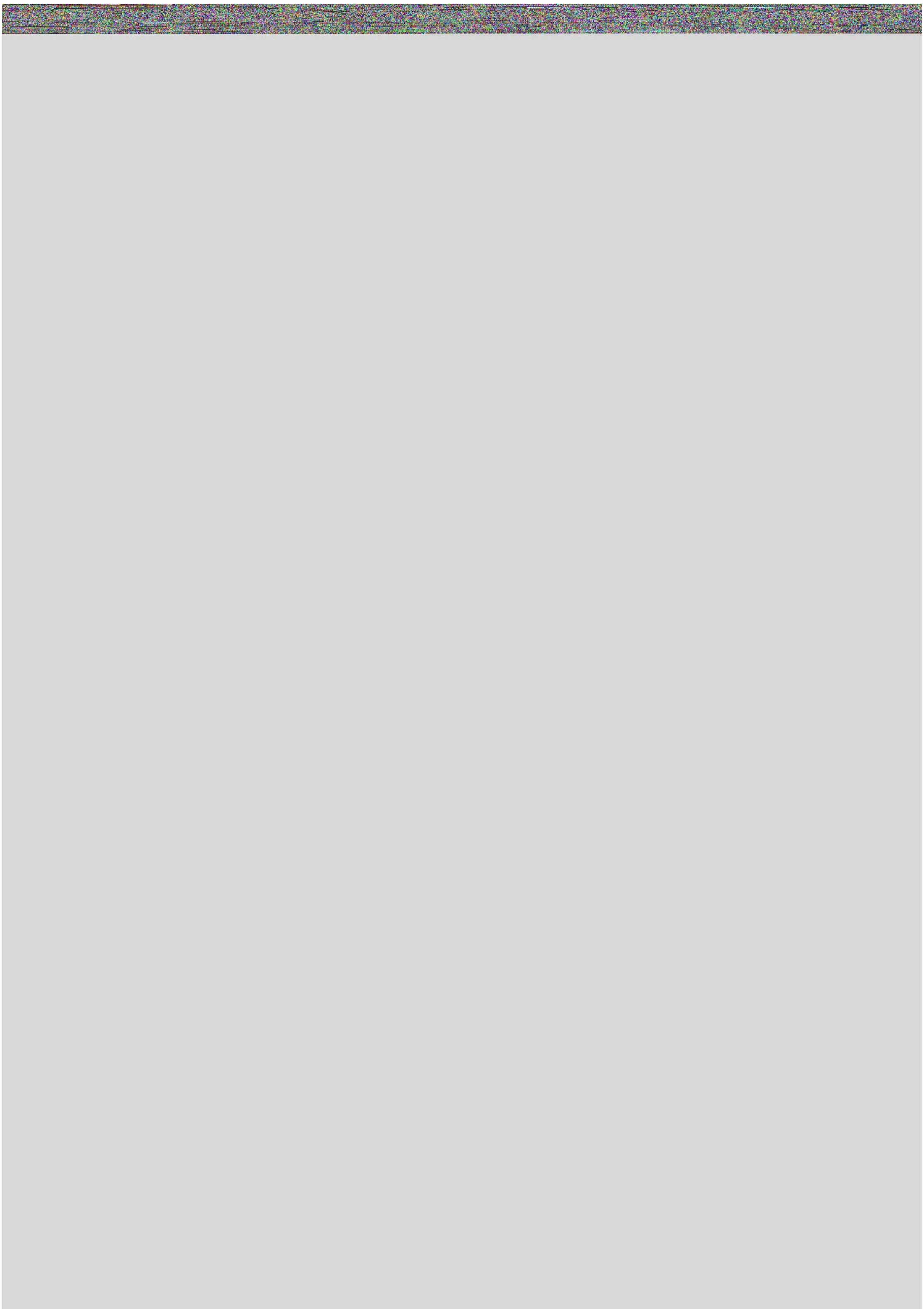


^{31}P NMR of Compound 4a



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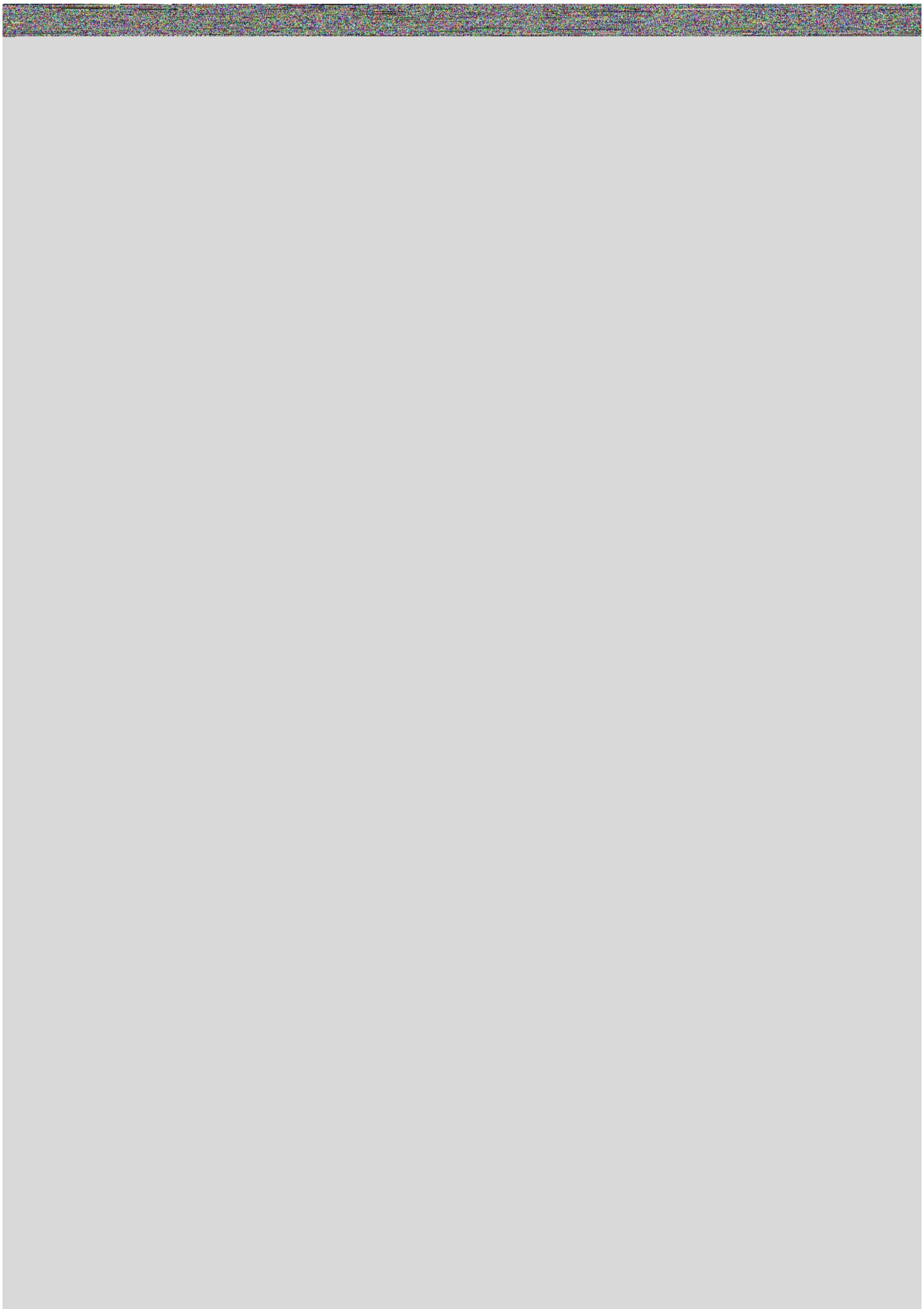

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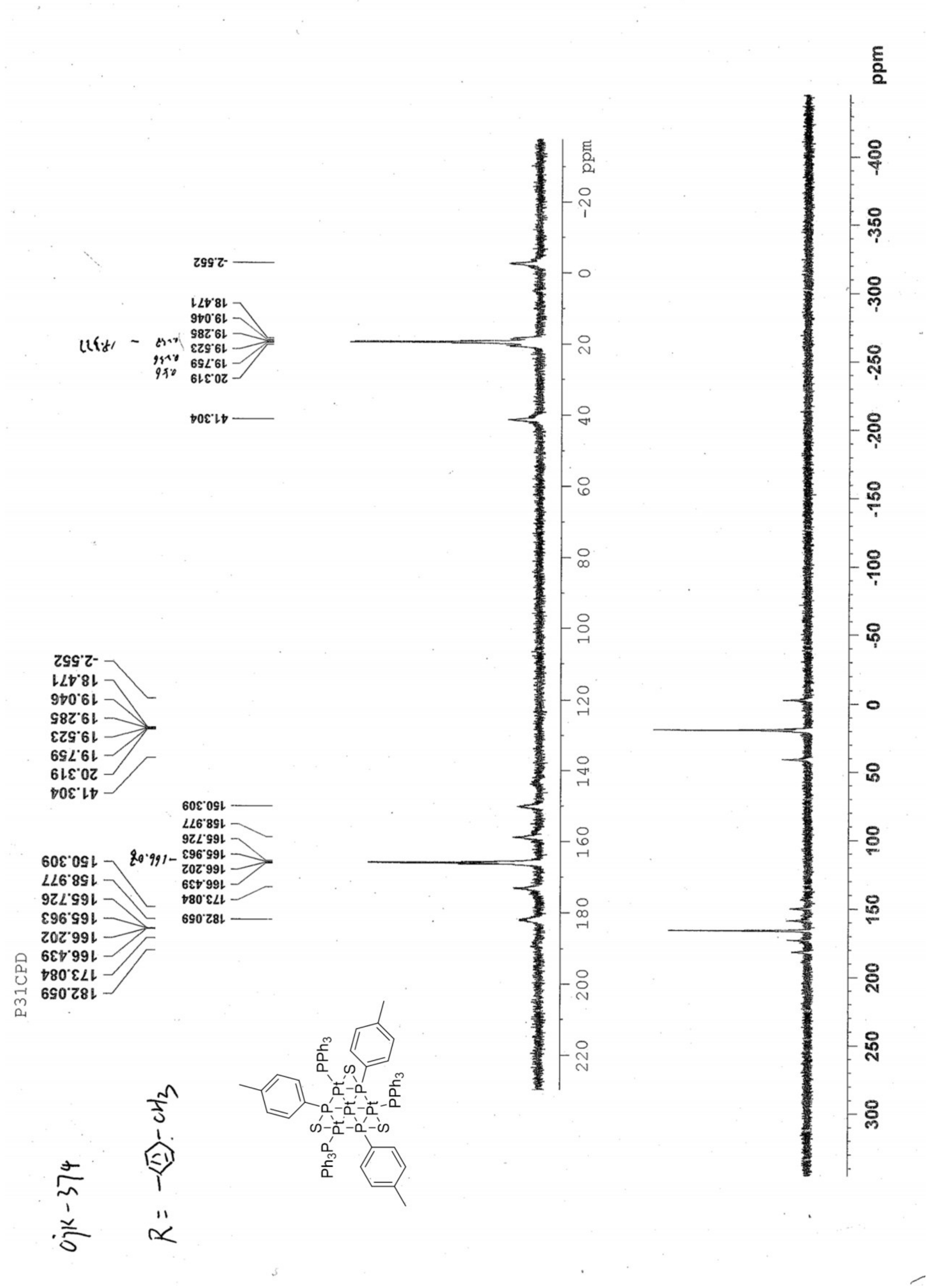

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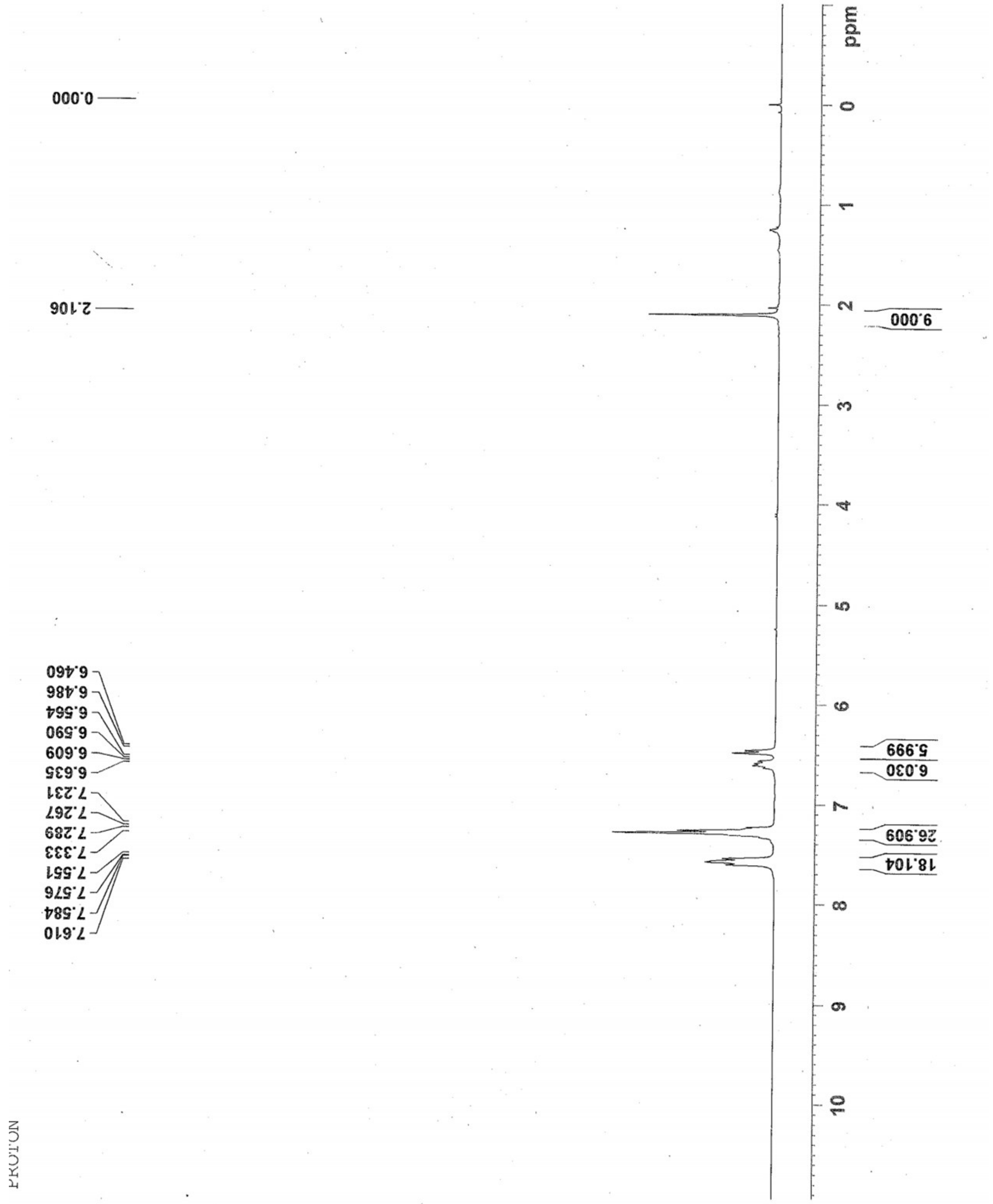

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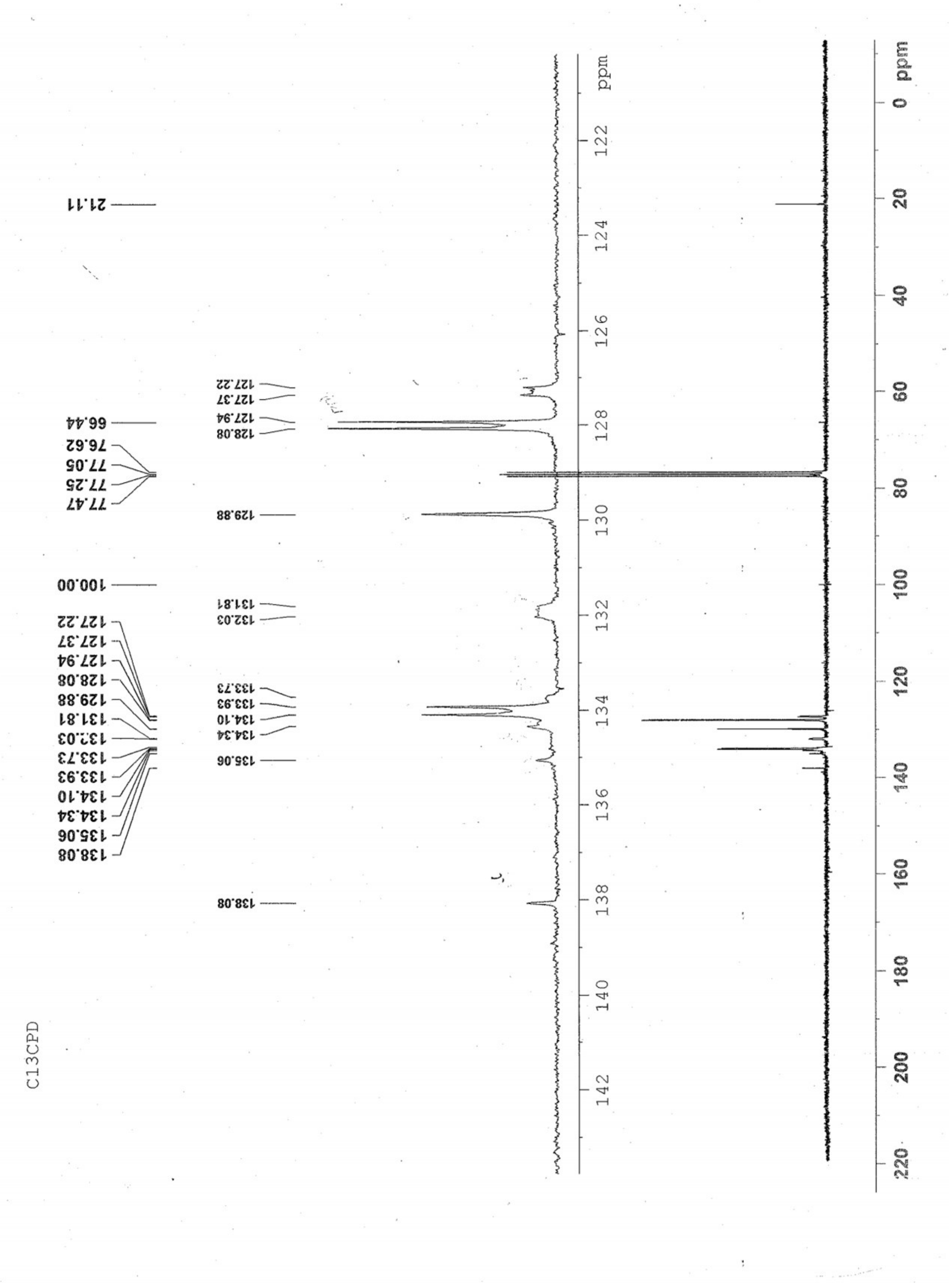

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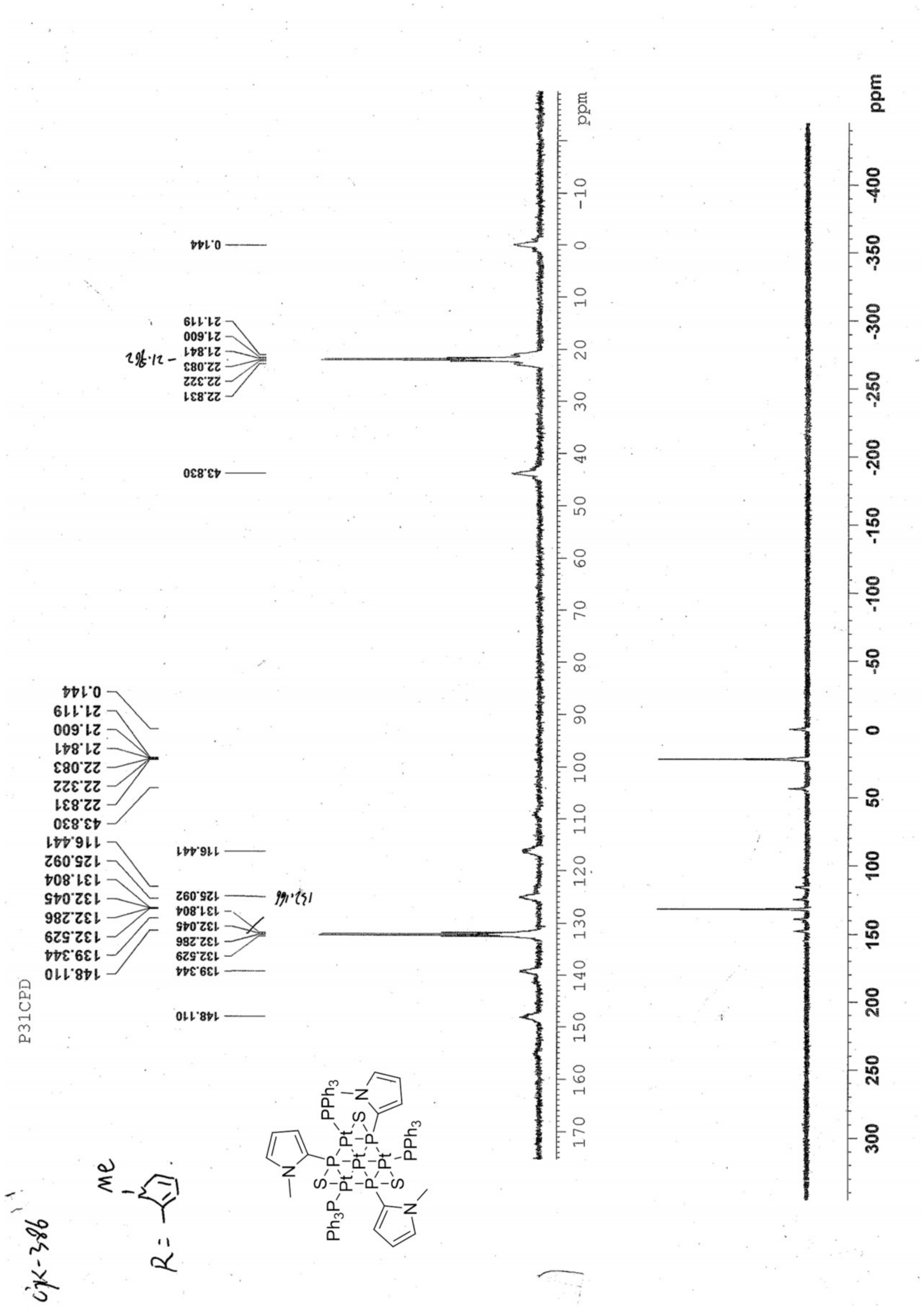

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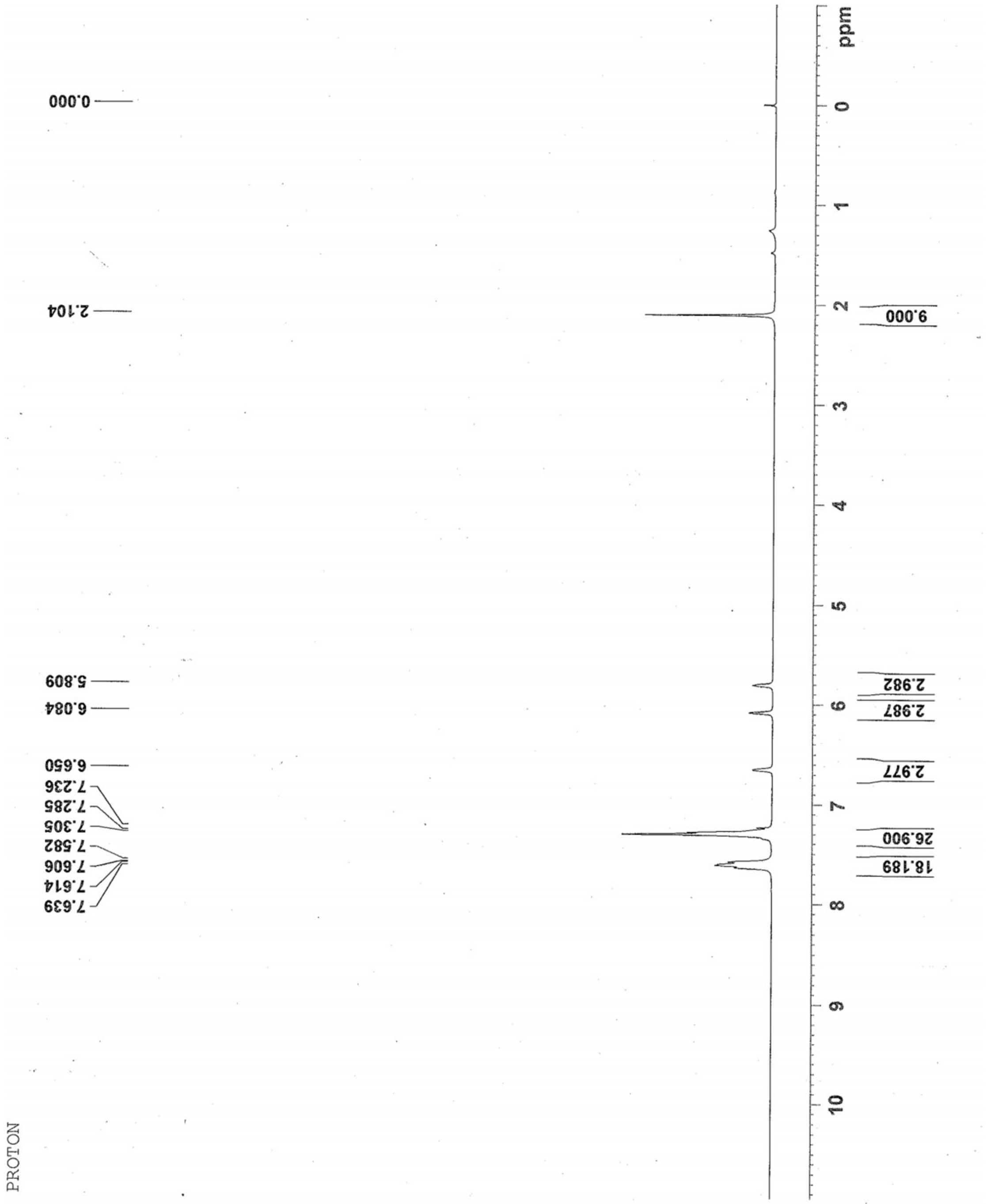

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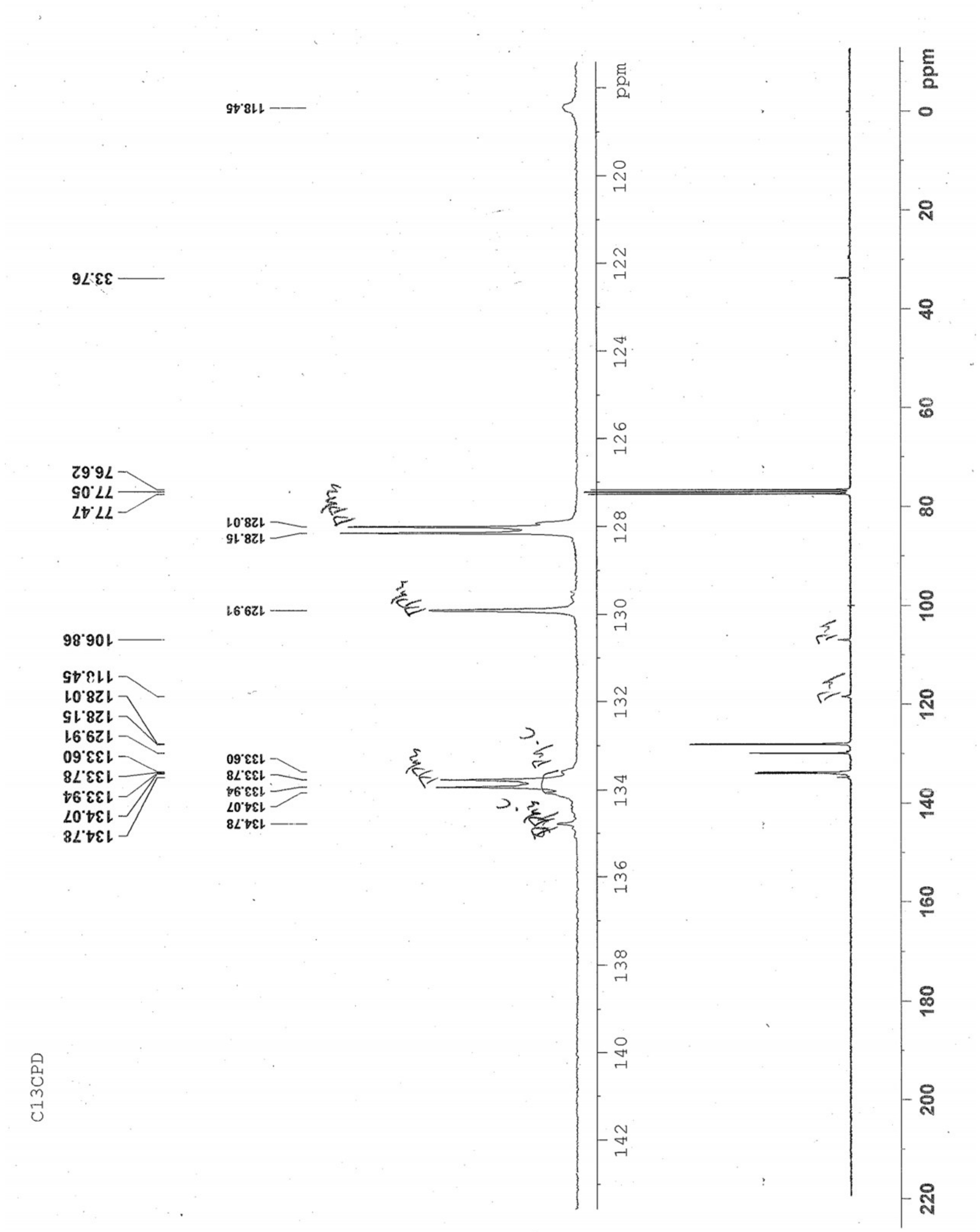

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