Supporting Information for

C-H and H-H Bond Activation via Ligand Dearomatization/Rearomatization of a PN^3P-Rhodium(I) Complex

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Experimental Section

General Procedures. All experiments (if not mentioned otherwise) with metal complexes were carried out under an atmosphere of dry argon in a glovebox or using standard Schlenk techniques. All glassware was rigorously dried. All solvents were distilled from sodium benzophenone ketyl prior to use. All other chemicals were commercially available and used as received. Ligand **1** was prepared according to the literature procedure (ref. 41). NMR spectra were recorded at 400 MHz (^{1}H), 100 MHz (^{13}C), and 162 MHz (^{31}P) using a Bruker Avance-400 NMR spectrometer, 500 MHz (^{1}H), 126 MHz (^{13}C), and 202 MHz (^{31}P) using a Bruker Avance-500 NMR spectrometer, and 600 MHz (^{1}H), 152 MHz (^{13}C), and 243 MHz (^{31}P) using a Bruker Avance-600 NMR spectrometer. All spectra were recorded at 23 °C. ^{1}H NMR chemical shifts were referenced to the residual hydrogen signals of the deuterated solvents (2.50 ppm, DMSO-d_6; 7.16 ppm, C_6D_6), and the ^{13}C NMR chemical shifts were referenced to the ^{13}C signals of the deuterated solvents (39.52 ppm, DMSO-d_6; 128.06 ppm, C_6D_6).

Reaction of ligand (1) with $[Rh(COD)_2Cl]_2$ to form $(PN^3P)Rh^ICl$ (2). A THF solution of **1** (10 mL, 715 mg, 1.80 mmol) was dropwise added to a stirred solution of $[Rh(COD)_2Cl]_2$ (444 mg, 0.90 mmol) in THF (10 mL). The resulting orange suspension was stirred overnight at 60 °C. The solvent was removed under vacuum, and the residue was washed with pentane, resulting in the analytically pure compound **2**. Yield: 888 mg (92%). ^{31}P{^{1}H} NMR (DMSO-d_6, 162 MHz): 107.89 (d, J_{Rh-P} = 153 Hz, 2P). ^{1}H NMR (DMSO-d_6, 400 MHz): 7.61 (s, 2H, N*H*), 7.12 (t, J_{H-H} = 8.0 Hz, 1H, Py H4), 6.12 (d, J_{H-H} = 8.0 Hz, 2H, Py H3,5), 1.35 (vt, J_{P-H} = 6.4 Hz, 36H, PC(CH_3)$_3$). ^{13}C NMR (DMSO-d_6, 126 MHz): 163.04 (PyC), 133.64 (PyC), 95.97 (PyC), 37.51 (P*C*(CH$_3$)$_3$), 28.42 (PC(*C*H$_3$)$_3$). Anal. Calcd for $C_{21}H_{41}ClN_3P_2Rh\cdot(C_4H_8O)$: C, 49.39; H, 8.12; N, 6.91. Found: C, 49.58; H, 8.53; N, 7.06.

Reaction of $(PN^3P)Rh^ICl$ (2) with benzene in the presence of $KN(SiMe_3)_2$ to form $(PN^3P)Rh^I(C_6H_5)$ (4). A benzene solution (2 mL) of $KN(SiMe_3)_2$ (21.0 mg, 0.10 mmol, 95% purity) was added to a stirred orange benzene suspension (3 mL) of **2** (53.6 mg, 0.10 mmol) under argon atmosphere. A considerable amount of red solid was precipitated and gradually consumed during 10 days at room temperature, giving a homogeneous red solution. The resulting mixture was evaporated, leaving a reddish-brown residue. The residue was extracted with pentane and filtered to remove KCl. The extract was dried in vacuum to give 48.2 mg (84% yield) of **4** as a reddish-brown solid. $^{31}P\{^1H\}$ NMR (C_6D_6, 162 MHz): 108.63 (d, J_{Rh-P} = 180 Hz, 2P). ^1H NMR (C_6D_6, 400 MHz): 8.12 (d, J_{H-H} = 7.2 Hz, 2H, Rh-Ph), 7.25 (t, J_{H-H} = 7.2 Hz, 2H, Rh-Ph), 6.99 (t, J_{H-H} = 7.2 Hz, 1H, Rh-Ph), 6.93 (t, J_{H-H} = 7.8 Hz, 1H, Py H4), 5.57 (d, J_{H-H} = 8.0 Hz, 2H, Py H3,5), 4.65 (s, 2H, N*H*), 1.24 (vt, J_{P-H} = 6.4 Hz, 36H, PC(C*H*$_3$)$_3$). ^{13}C NMR (C_6D_6, 126 MHz): 168.55 (dt, J_{Rh-C} = 32 Hz, J_{P-C} = 14 Hz, Rh-*C*), 159.96 (s, Py), 143.18 (s, Ph), 134.18 (s, Py), 125.07 (s, Ph), 119.12 (s, Py), 96.04 (s, Ph), 38.34 (br, *C*(CH$_3$)$_3$), 28.90 (br, C(*C*H$_3$)$_3$). Anal. Calcd for $C_{27}H_{46}N_3P_2Rh\cdot(0.5C_6H_6)$: C, 58.44; H, 8.01; N, 6.81. Found: C, 58.37; H, 8.35; N, 7.24.

Reaction of $(PN^3P)Rh^ICl$ (2) with CO in the presence of ^{t}BuOK to form dearomatized $(PN^3P)Rh^I(CO)$ (5). To a THF (4 mL) solution of **2** (53.6 mg, 0.10 mmol) was added ^{t}BuOK (11.2 mg, 0.10 mmol). Then the solution was degassed and refilled with CO at room temperature, resulting in an immediate color change to green. The solution was evaporated, leaving a green residue. The residue was extracted with pentane and filtered to remove KCl. The extract was dried in vacuum, giving 49.4 mg (94% yield) of **5** as green solid. IR (thin film): ν_{CO} 1952 cm^{-1}. $^{31}P\{^1H\}$ NMR (C_6D_6, 162 MHz): 130.55 (dd (AB), J_{P-P} = 248 Hz, J_{Rh-P} = 124 Hz, 1P), 121.58 (dd (AB), J_{P-P} = 248 Hz, J_{Rh-P} = 126 Hz, 1P). ^1H NMR (C_6D_6, 400 MHz): 6.86 (t, J_{H-H} = 8.0 Hz, 1H, Py H4), 6.70 (d, J_{H-H} = 8.4 Hz, 1H, Py*H*), 5.11 (d, J_{H-H} = 7.2 Hz, 1H, Py*H*), 4.16 (s, 1H, N*H*), 1.51 (s, 9H, PC(C*H*$_3$)$_3$), 1.48 (s, 9H, PC(C*H*$_3$)$_3$), 1.05 (s, 9H, PC(C*H*$_3$)$_3$), 1.01 (s, 9H, PC(C*H*$_3$)$_3$). ^{13}C NMR (C_6D_6, 126 MHz): 200.08 (dt, J_{Rh-C} = 69.0 Hz, J_{P-C} = 11.3 Hz, *C*O), 173.52 (s, Py), 160.49 (m, Py), 138.62 (s, Py C4), 106.09 (d, J_{P-C} = 23.2 Hz, Py), 86.04 (s, Py), 38.30 (s, P*C*(CH$_3$)$_3$), 37.73 (s, P*C*(CH$_3$)$_3$), 28.94 (s, PC(*C*H$_3$)$_3$), 28.18 (s, PC(*C*H$_3$)$_3$). Anal. Calcd for $C_{22}H_{40}N_3OP_2Rh$: C, 50.10; H, 7.64; N, 7.97. Found: C, 49.89; H, 7.75; N, 7.87.

Reaction of $(PN^3P)Rh^I(CO)$ (5) with HCO_2H to form $[(PNP)Rh^I(CO)][HCOO]$ (5a). To a solution of 5 (10.5 mg, 0.020 mmol) in benzene (0.5 mL) was added excess amount of HCOOH, accompanying with a color change from green to light yellow. The solution was evaporated to dryness, giving 11.0 mg (96% yield) of **5a** as light yellow solid. IR (thin film): ν_{CO} 1969 cm^{-1}. $^{31}P\{^1H\}$ NMR (DMSO-d_6, 162 MHz): 131.95 (d, J_{Rh-P} = 126 Hz, 2P). ^1H NMR (DMSO-d_6, 400 MHz): 8.86 (s, 2H, NH), 8.26 (s, 1H, HCO), 7.54 (t, J_{H-H} = 8.0 Hz, 1H, Py H4), 6.48 (d, J_{H-H} = 8.0 Hz, 2H, Py H3,5), 1.35 (vt, J_{P-H} = 7.6 Hz, 36H, PC(C*H*$_3$)$_3$). ^{13}C NMR (DMSO-d_6, 126 MHz): 195.98 (dt, J_{Rh-C} = 68.4 Hz, J_{P-C} = 13.0 Hz, *C*O), 164.20 (s, H*C*O$_2$), 162.73 (t, J_{P-C} = 7.1 Hz, Py), 142.86 (s, Py), 99.34 (s, Py), 38.47 (t, J_{P-C} = 10.0 Hz, P*C*(CH$_3$)$_3$), 27.95 (s, PC(*C*H$_3$)$_3$). Anal. Calcd for $C_{23}H_{42}N_3O_3P_2Rh\cdot 2(CH_2O_2)$: C, 45.12; H, 6.97; N, 6.31. Found: C, 45.29; H, 7.21; N, 6.54.

Reaction of (PN^3P)Rh^ICl (2) with H_2 in the presence of KH to form (PN^3P)Rh^IH (6). To a solution of **2** (53.6 mg, 0.10 mmol) in THF (4 mL) was added KH (4.0 mg, 0.10 mmol). Then the solution was degassed and refilled with H_2 at room temperature, resulting in an immediate color change to dark reddish brown. The solution was evaporated, leaving a dark reddish brown residue. The residue was extracted with pentane and filtered to remove KCl. The extract was dried in vacuum, giving 42.5 mg (85% yield) of **6** as reddish brown solid. $^{31}P\{^1H\}$ NMR (DMSO-d_6, 162 MHz): 135.03 (d, J_{Rh-P} = 168 Hz, 2P). ^1H NMR (DMSO-d_6, 400 MHz): 7.36 (s, NH, 2H), 7.11 (t, J_{H-H} = 7.8 Hz, 1H, Py H4), 6.14 (d, J_{H-H} = 7.8 Hz, 2H, Py H3,5), 1.24 (vt, J_{P-H} = 6.4 Hz, 36H, $PC(CH_3)_3$), −11.60 (dt, J_{Rh-H} = 25.2 Hz, J_{P-H} = 22.8 Hz, 1H, Rh-*H*). ^{13}C NMR (DMSO-d_6, 152 MHz): 160.64 (PyC), 133.34 (PyC), 95.44 (PyC), 36.26 ($PC(CH_3)_3$), 29.10 ($PC(CH_3)_3$). Anal. Calcd for $C_{21}H_{42}N_3P_2Rh$: C, 50.30; H, 8.44; N, 8.38. Found: C, 50.20; H, 7.78; N, 7.93.

Experiments to confirm the H_2 activation:

Reaction of (PN^3P)Rh^IH (6) with D_2O.

When hydride **6** was dissolved in a THF solution of D_2O, Rh-H/Rh-D exchange was observed:
In a J-Young tube, a THF solution (0.5 mL) of **6** (5.0 mg, 0.010 mmol) under an argon atmosphere was added D_2O (10 μL) and the mixture was kept overnight at rt. Examination of the mixture by $^2H\{^1H\}$NMR displayed a signal at −11.32 ppm, indicating the deuterium incorporation. Then THF was removed under reduced pressure and the residue was dissolved in DMSO-d_6 (0.5 mL). The ^1H NMR spectrum indicated that the Rh-*H* signal integrated at 80% of its normal intensity.

Reaction of (PN^3P)Rh^IH (6) with D_2.

Addition of D_2 to the proposed "intermediate **3**" was observed:
In a J-Young tube, a THF solution (0.5 mL) of **6** (5.0 mg, 0.010 mmol) under an argon atmosphere was injected with excess of dry D_2 and the mixture was kept overnight at rt. Examination of the mixture by $^2H\{^1H\}$NMR displayed a signal at −11.26 ppm, indicating the deuterium incorporation.

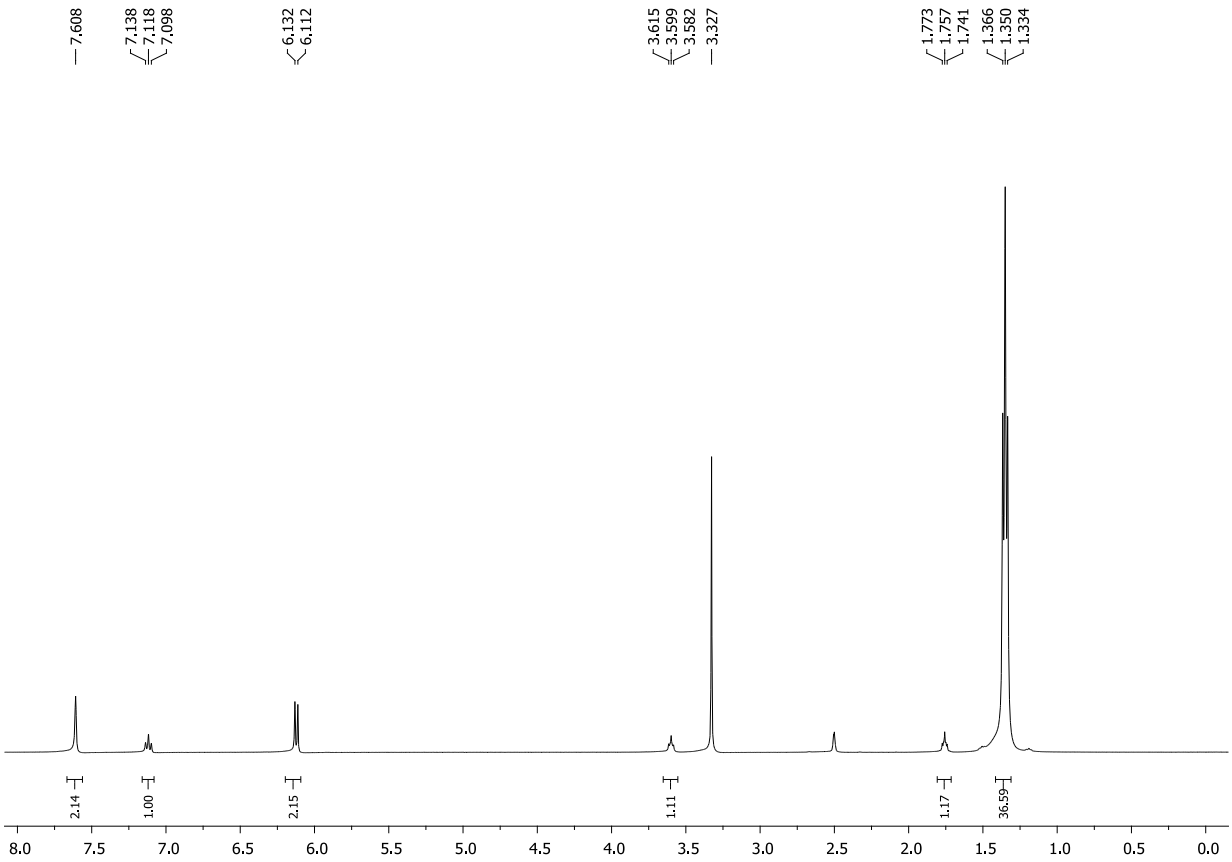


Figure S1 ^{1}H NMR spectrum of **2** (DMSO-d_6, 400 MHz).

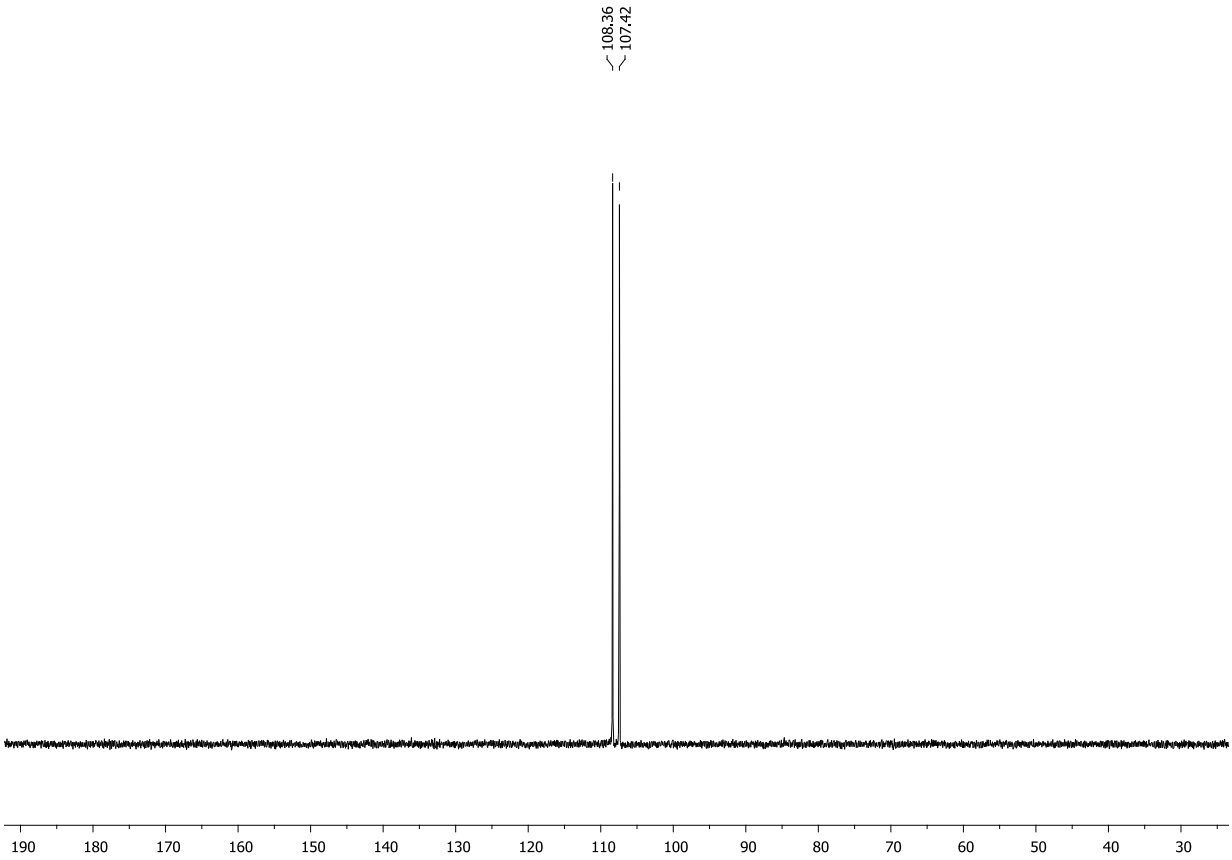


Figure S2 ^{31}P NMR spectrum of **2** (DMSO-d_6, 162 MHz).

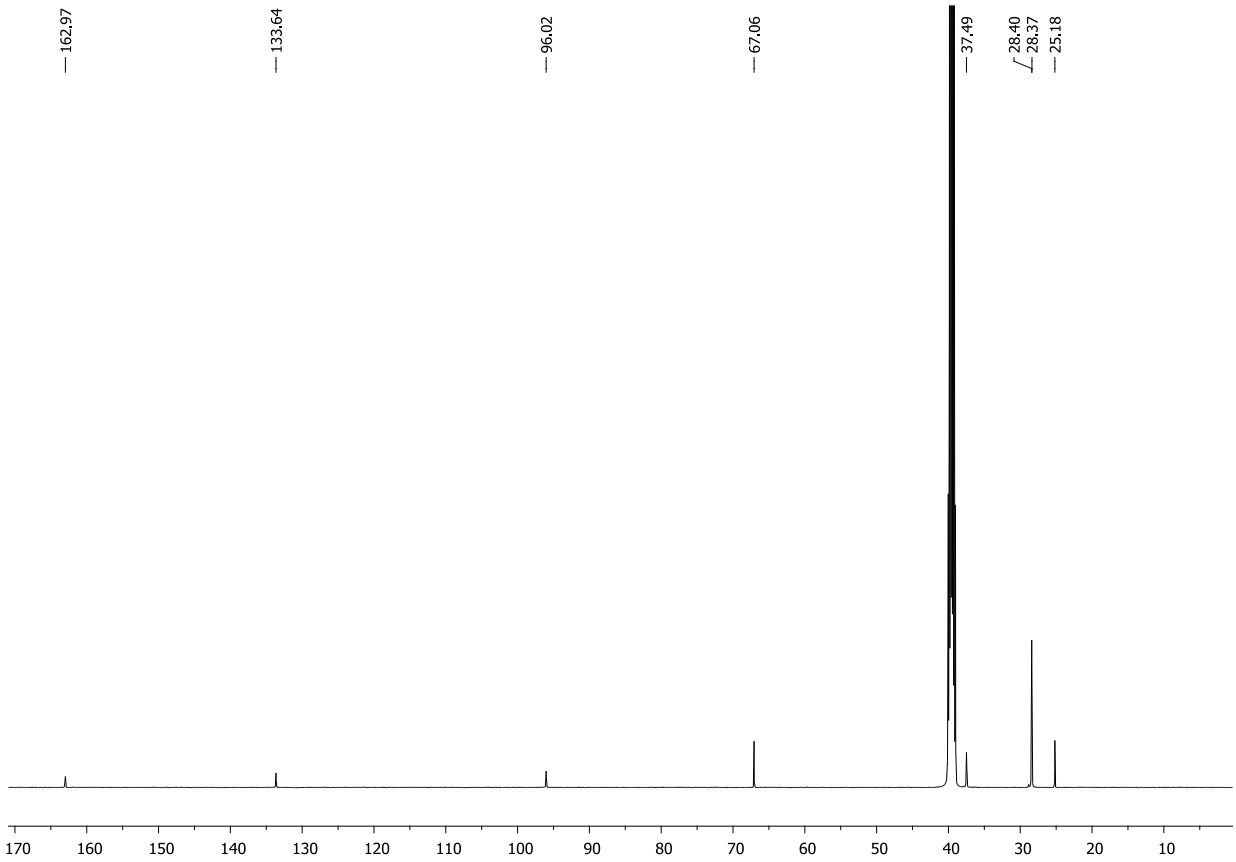


Figure S3 ^{13}C NMR spectrum of **2** (DMSO-d_6, 126 MHz).

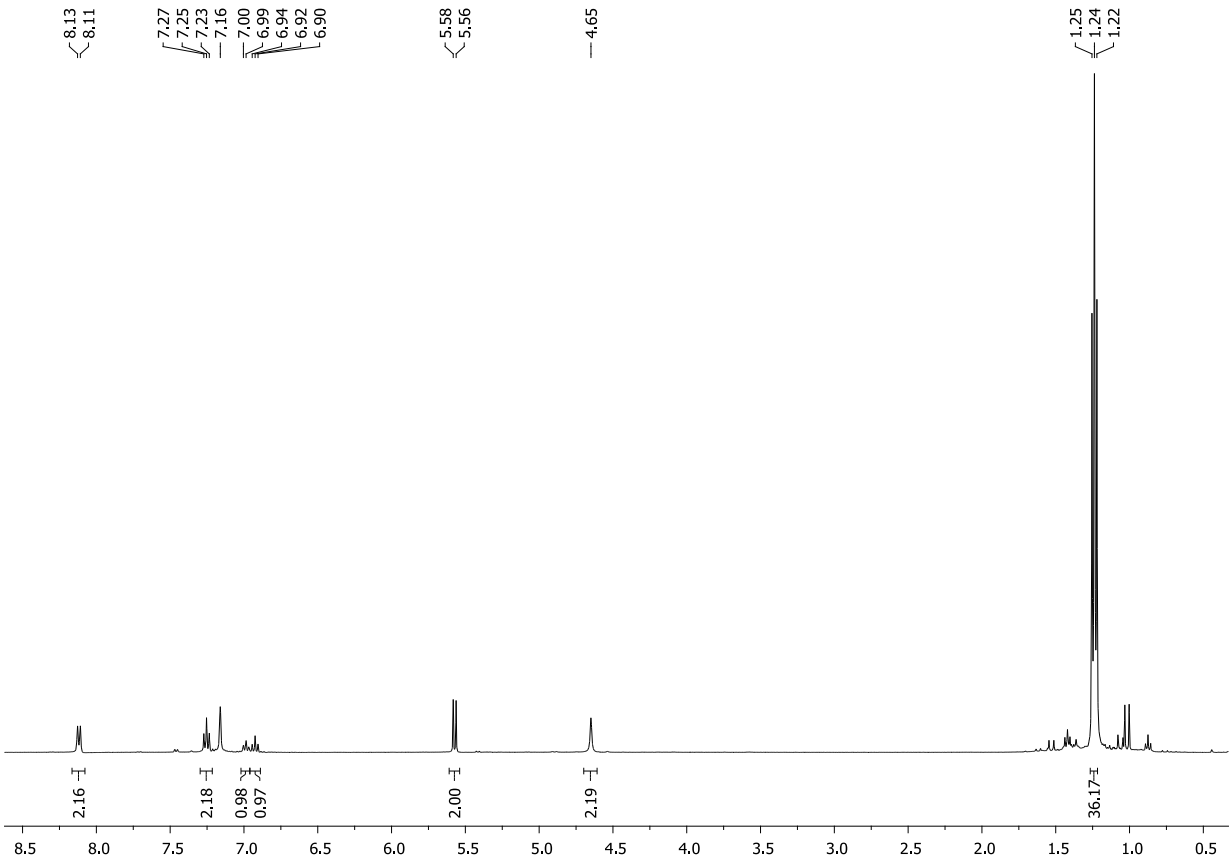


Figure S4 ^{1}H NMR spectrum of **4** (C_6D_6, 400 MHz).

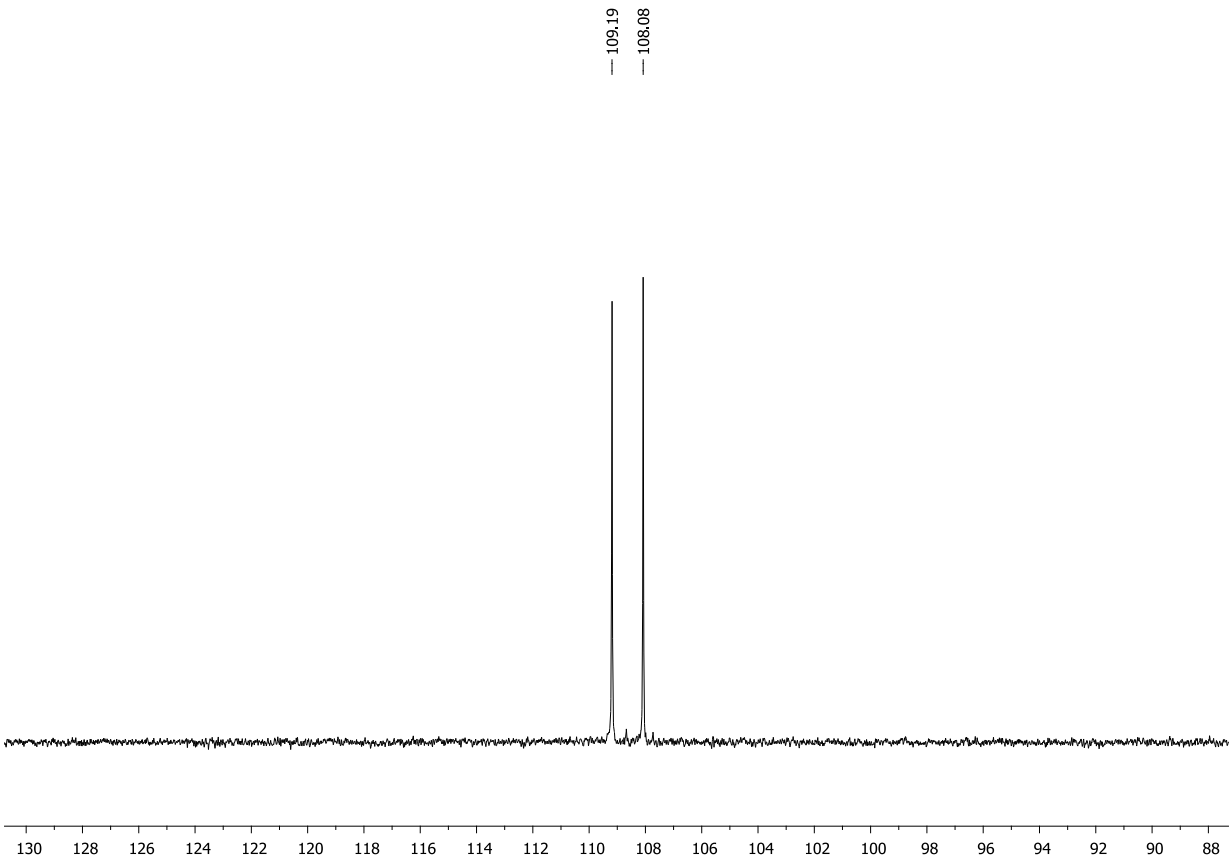


Figure S5 ^{31}P NMR spectrum of **4** (C_6D_6, 162 MHz).

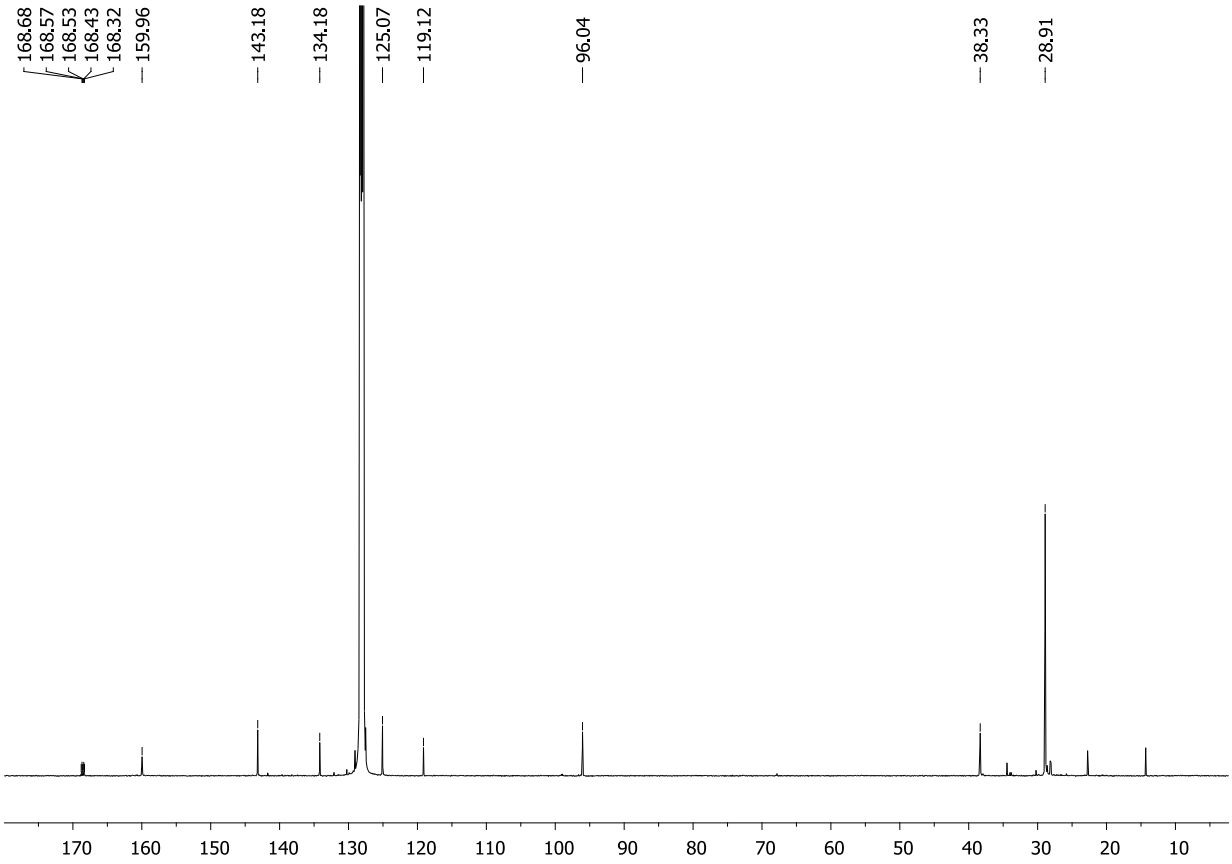


Figure S6 ^{13}C NMR spectrum of **4** (C_6D_6, 126 MHz).

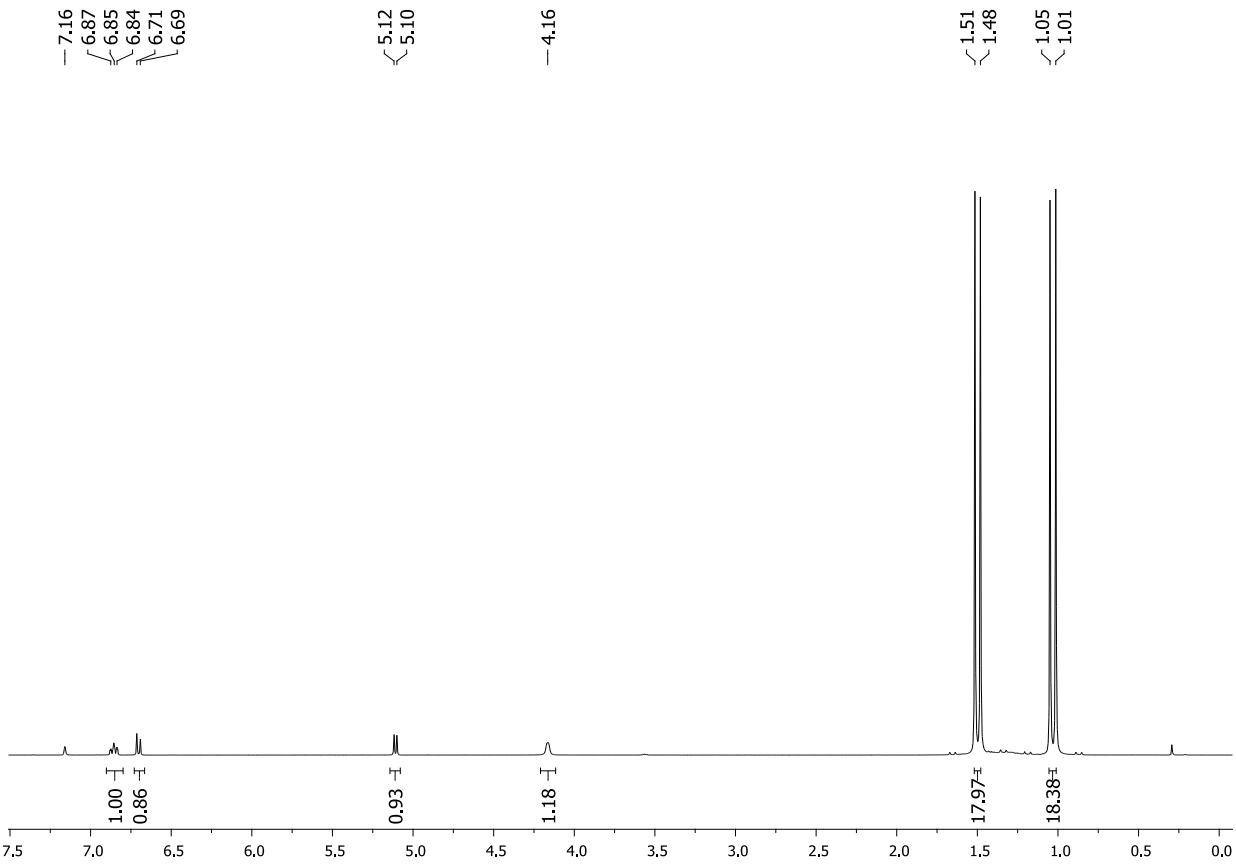


Figure S7 ^{1}H NMR spectrum of **5** (C_6D_6, 400 MHz).

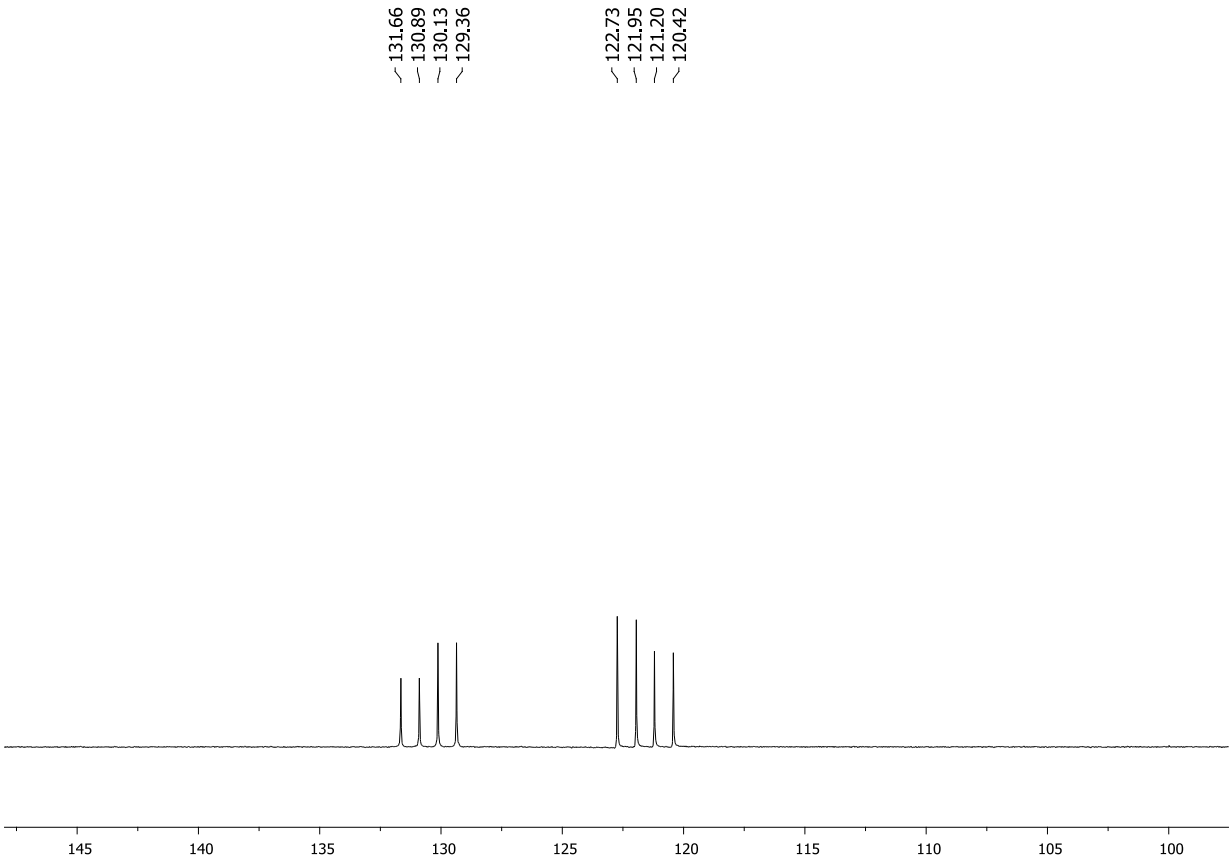


Figure S8 ^{31}P NMR spectrum of **5** (C_6D_6, 162 MHz).

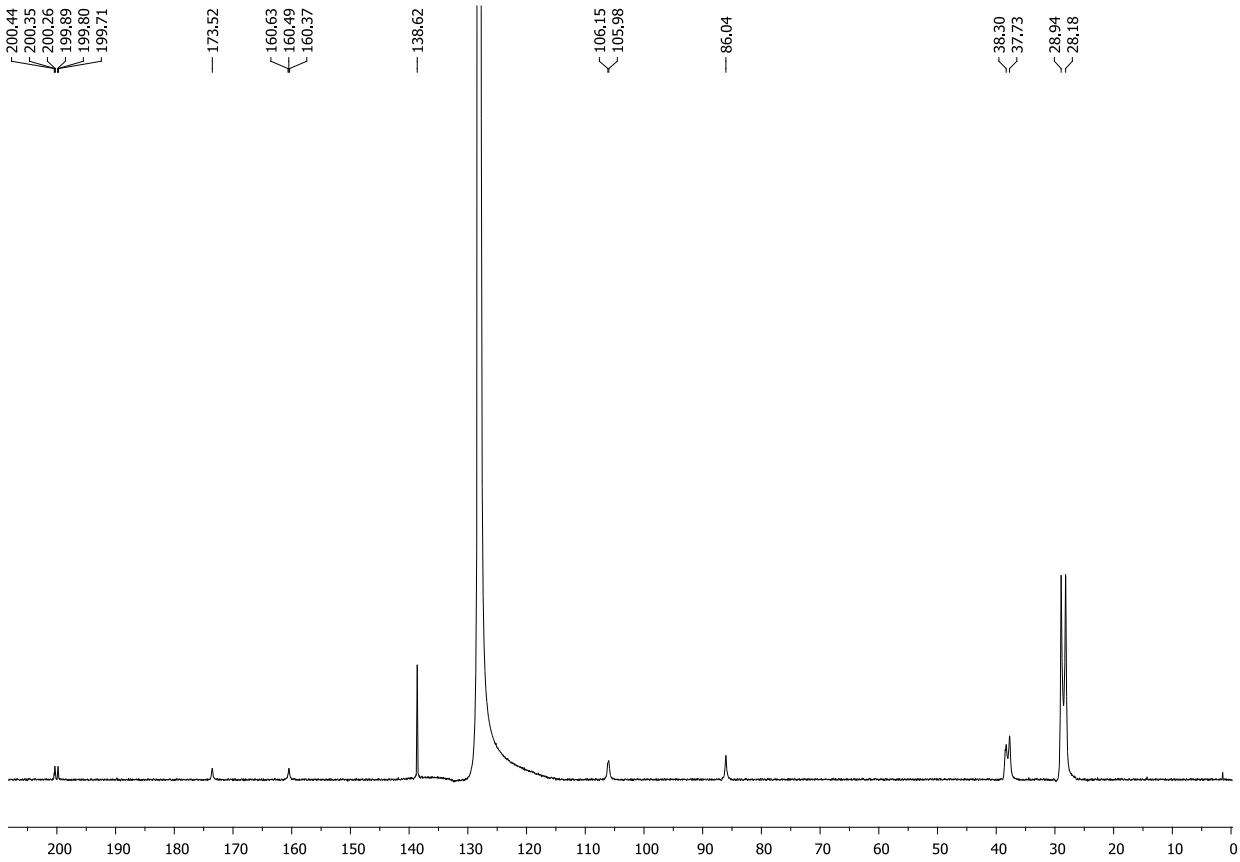


Figure S9 ^{13}C NMR spectrum of **5** (C_6D_6, 126 MHz)

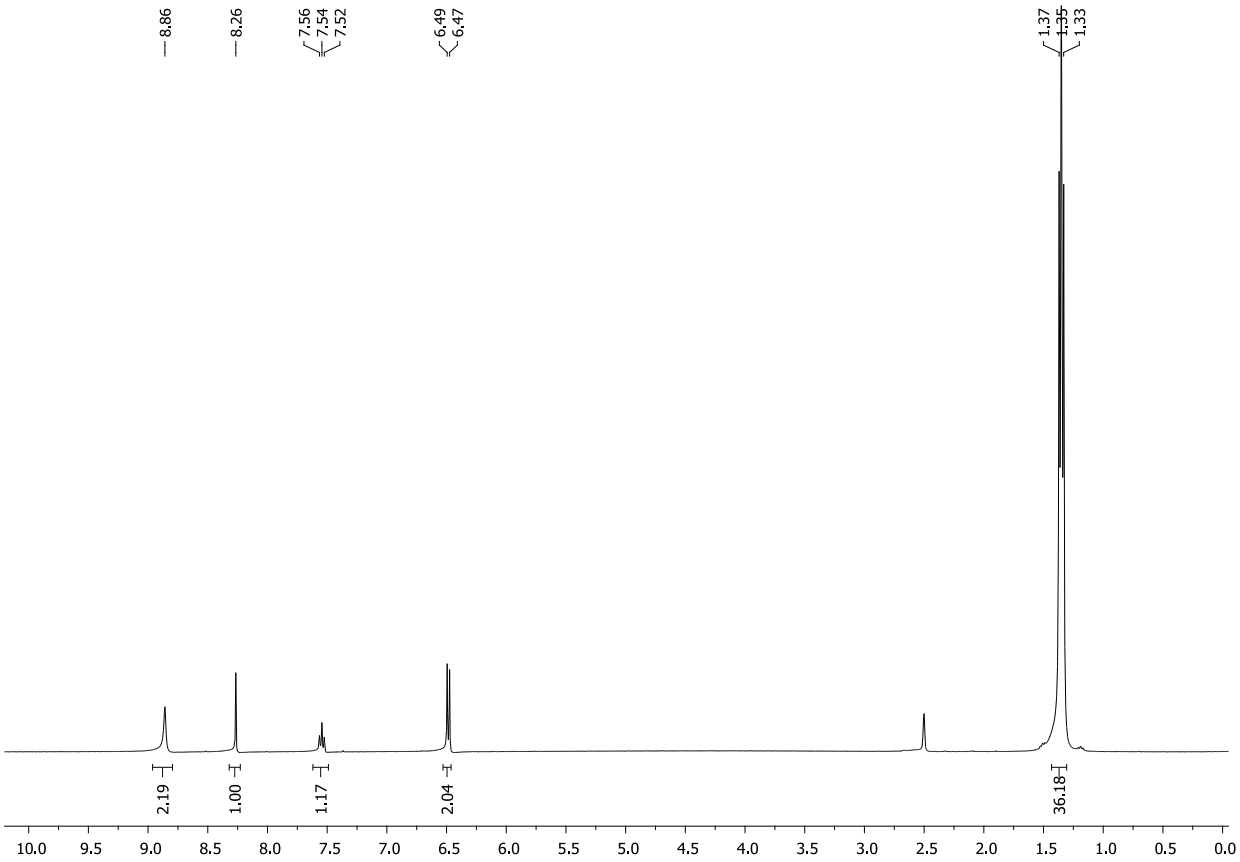


Figure S10 ^{1}H NMR spectrum of **5a** (DMSO-d_6, 400 MHz).

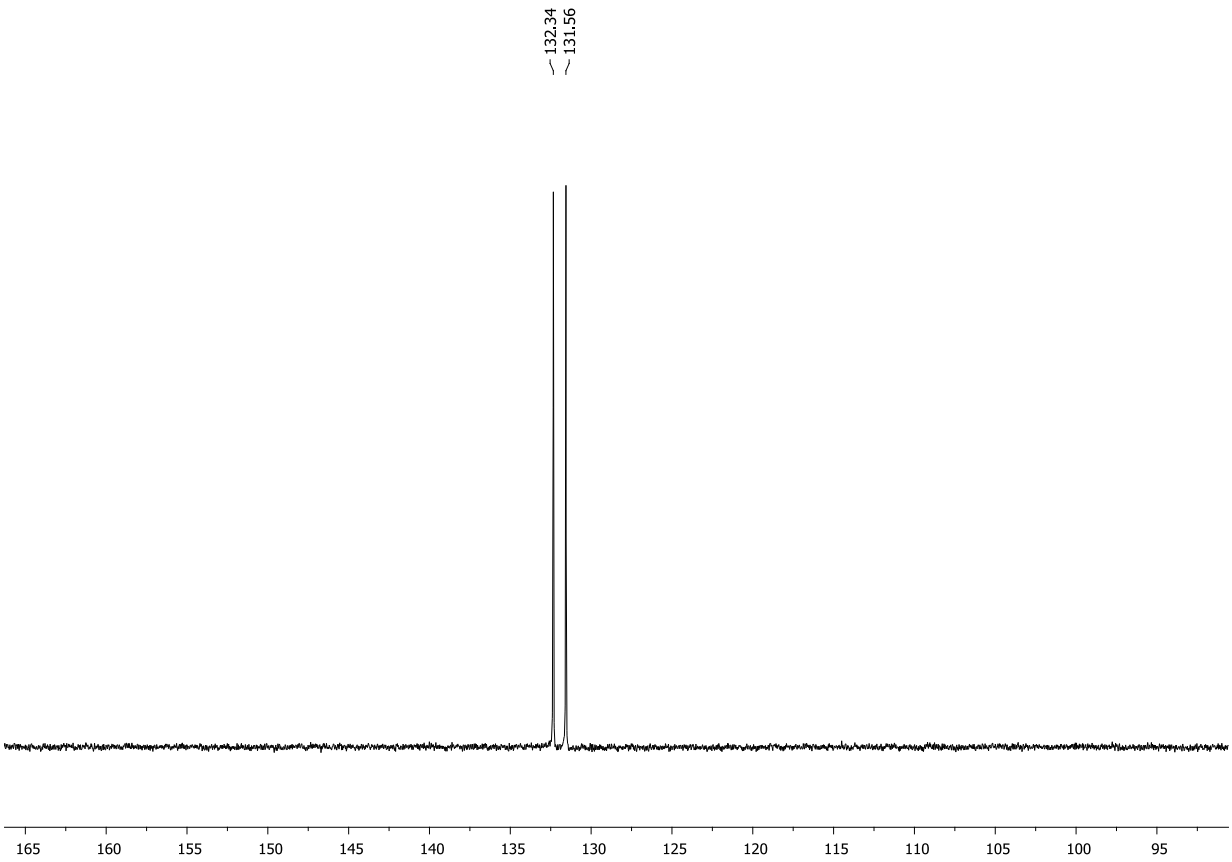


Figure S11 ^{31}P NMR spectrum of **5a** (DMSO-d_6, 162 MHz).

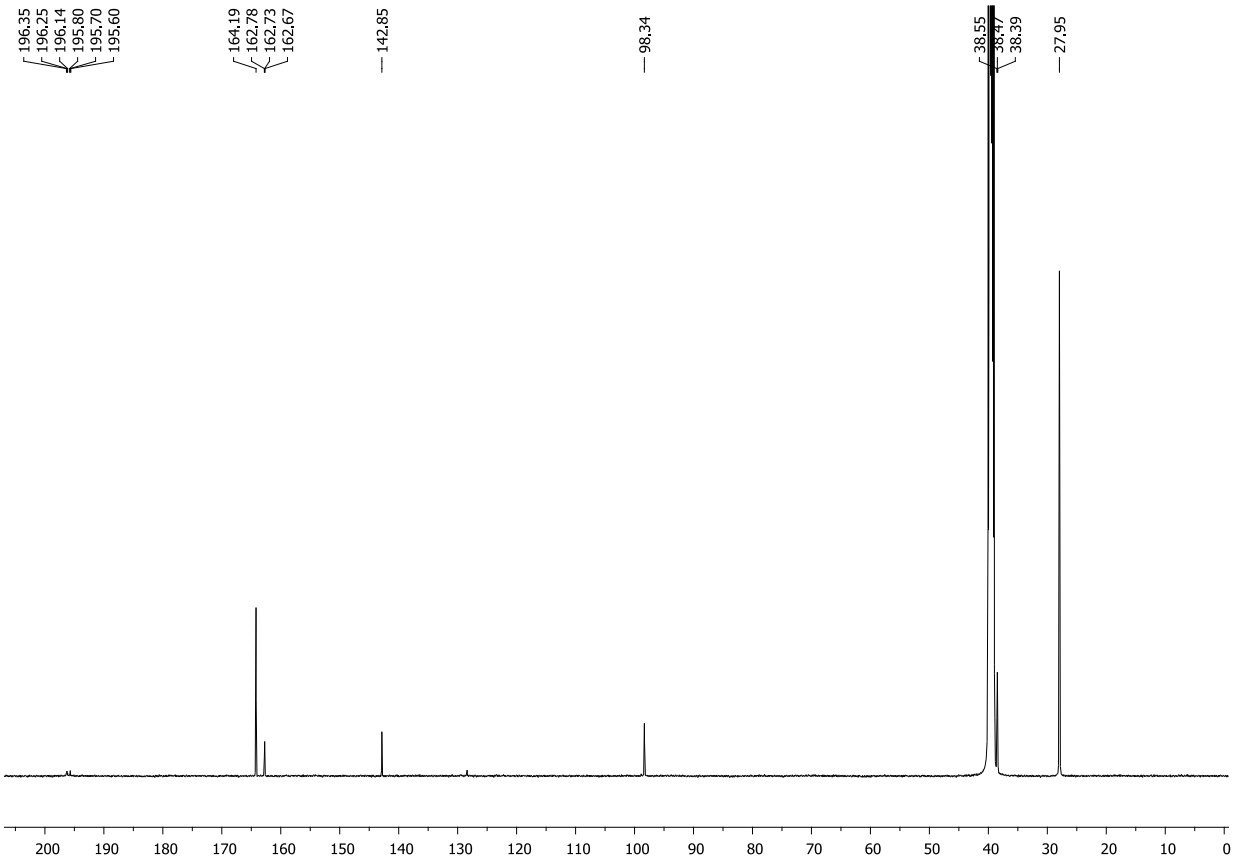


Figure S12 ^{13}C NMR spectrum of **5a** (C_6D_6, 126 MHz).

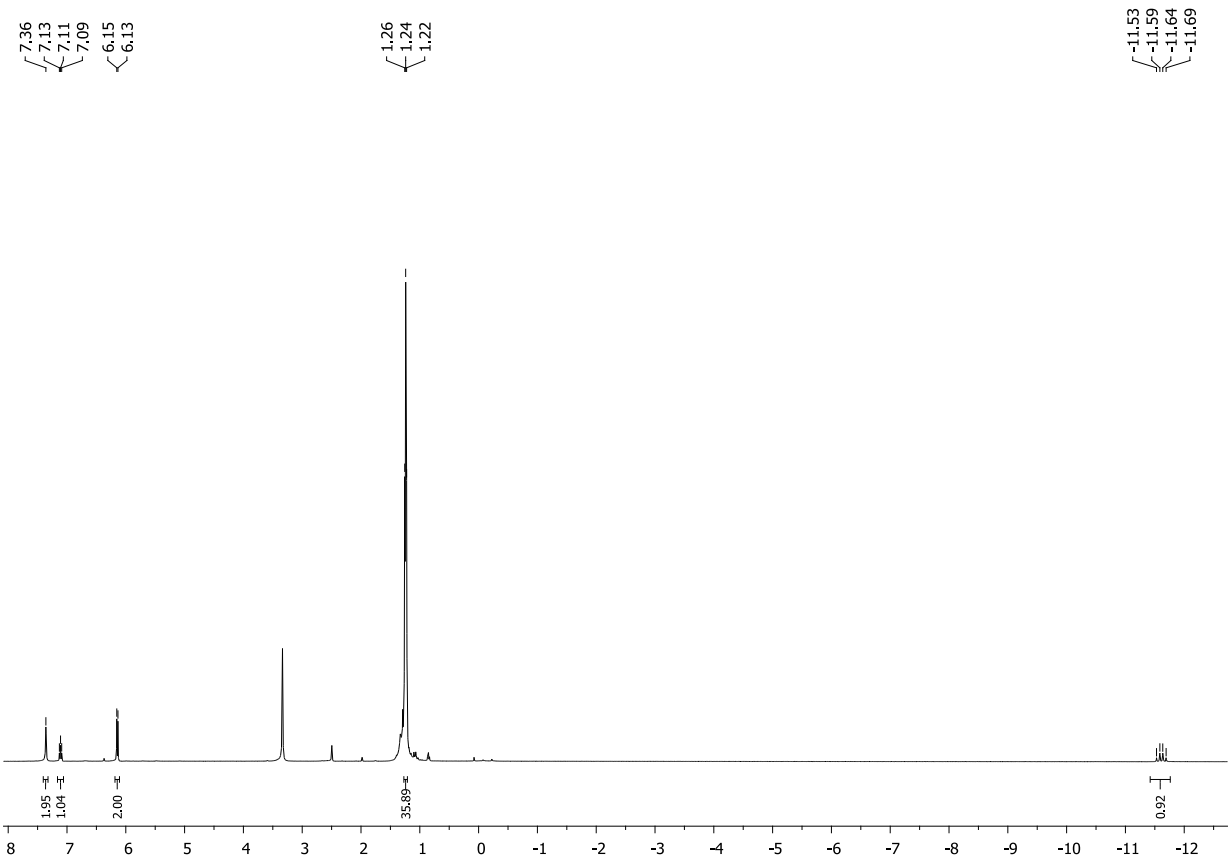


Figure S13 ^{1}H NMR spectrum of **6** (DMSO-d_6, 400 MHz).

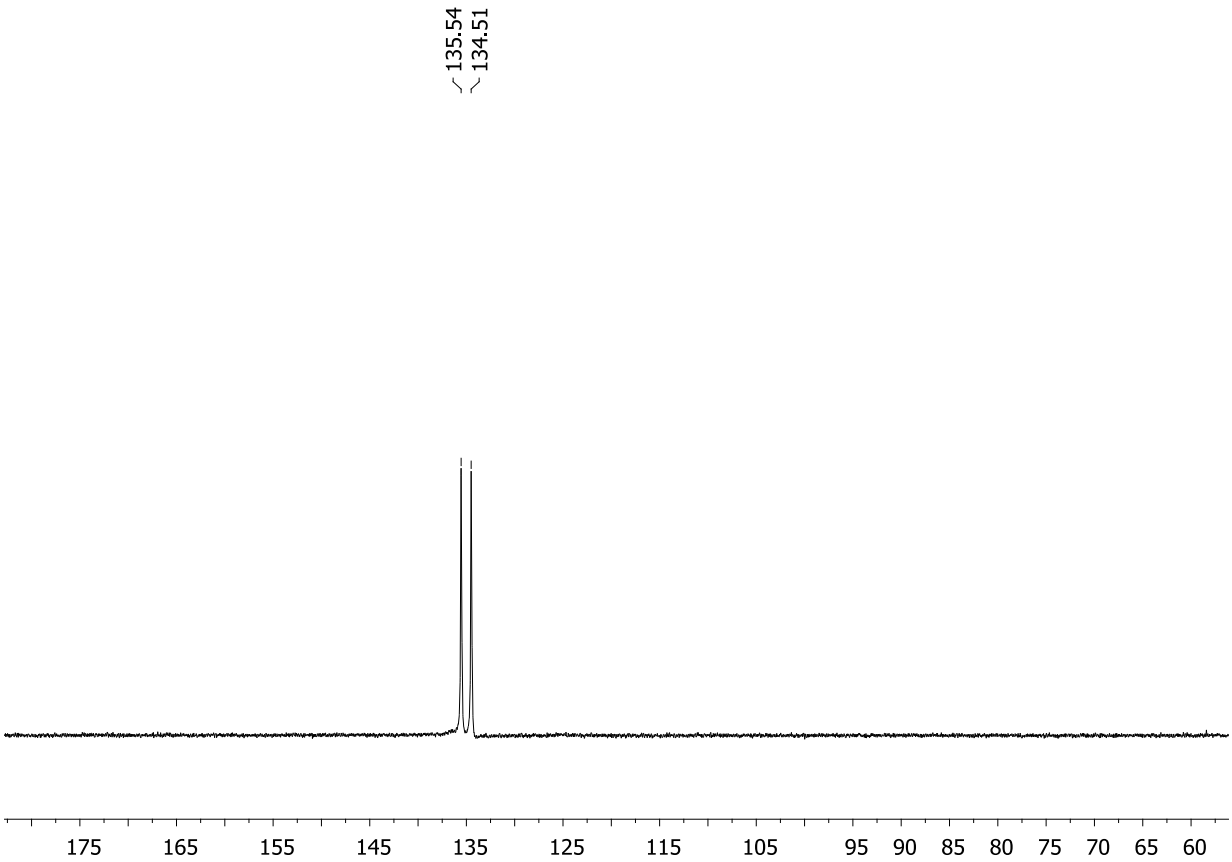


Figure S14 ^{31}P NMR spectrum of **6** (DMSO-d_6, 162 MHz).

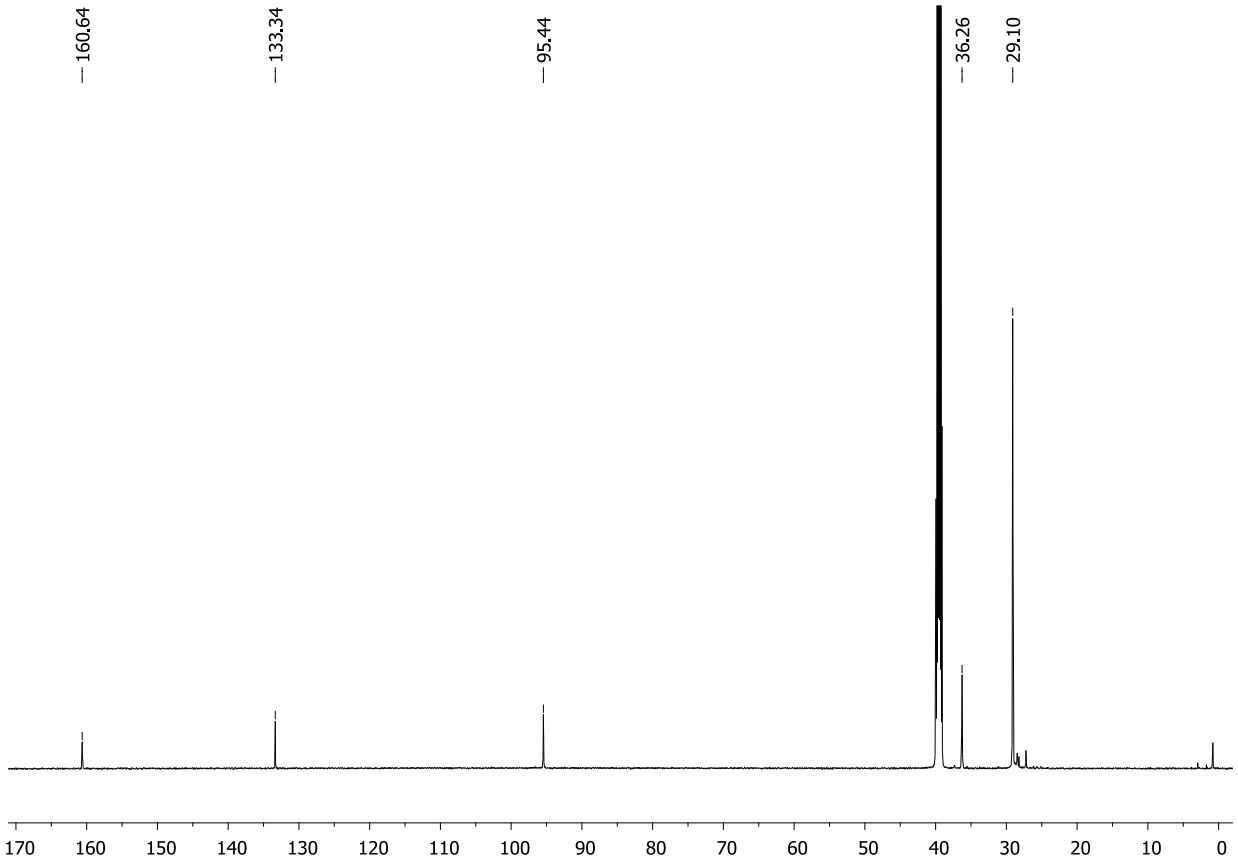


Figure S15 ^{13}C NMR spectrum of **6** (DMSO-d_6, 152 MHz).

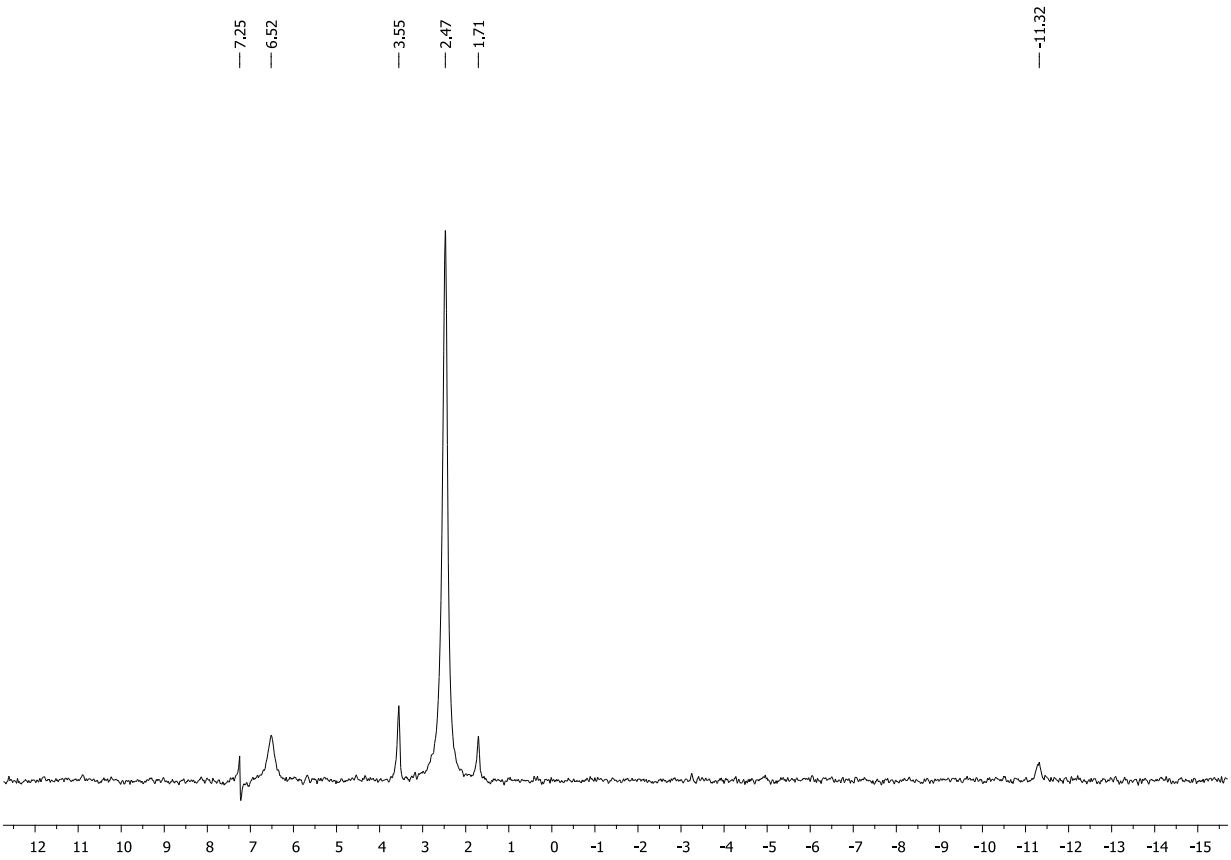


Figure S16 ^{2}D NMR spectrum of **6** with D_2O (THF, 600 MHz, 2000 scan times).

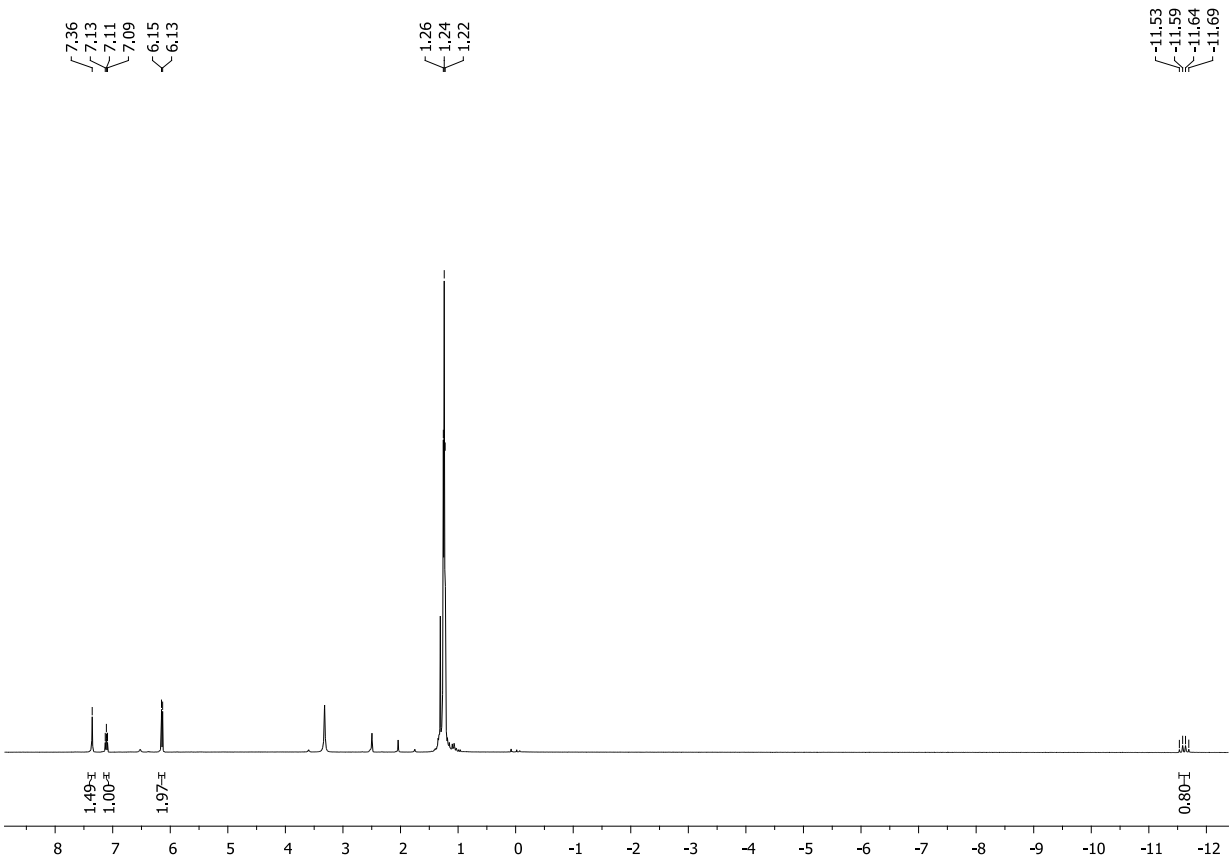


Figure S17 ^{1}H NMR spectrum of **6** with D_2O (DMSO-d_6, 400 MHz).

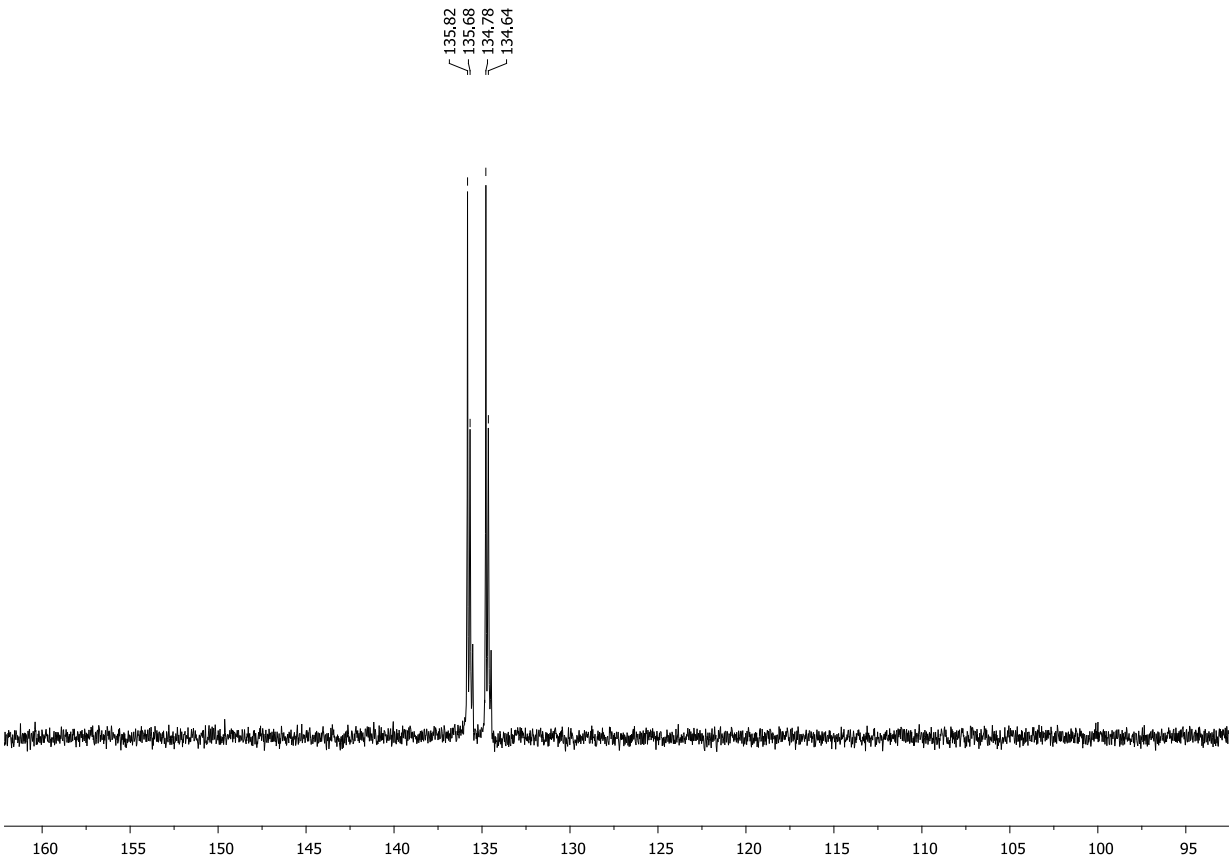


Figure S18 ^{31}P NMR spectrum of **6** with D_2O (DMSO-d_6, 162 MHz).

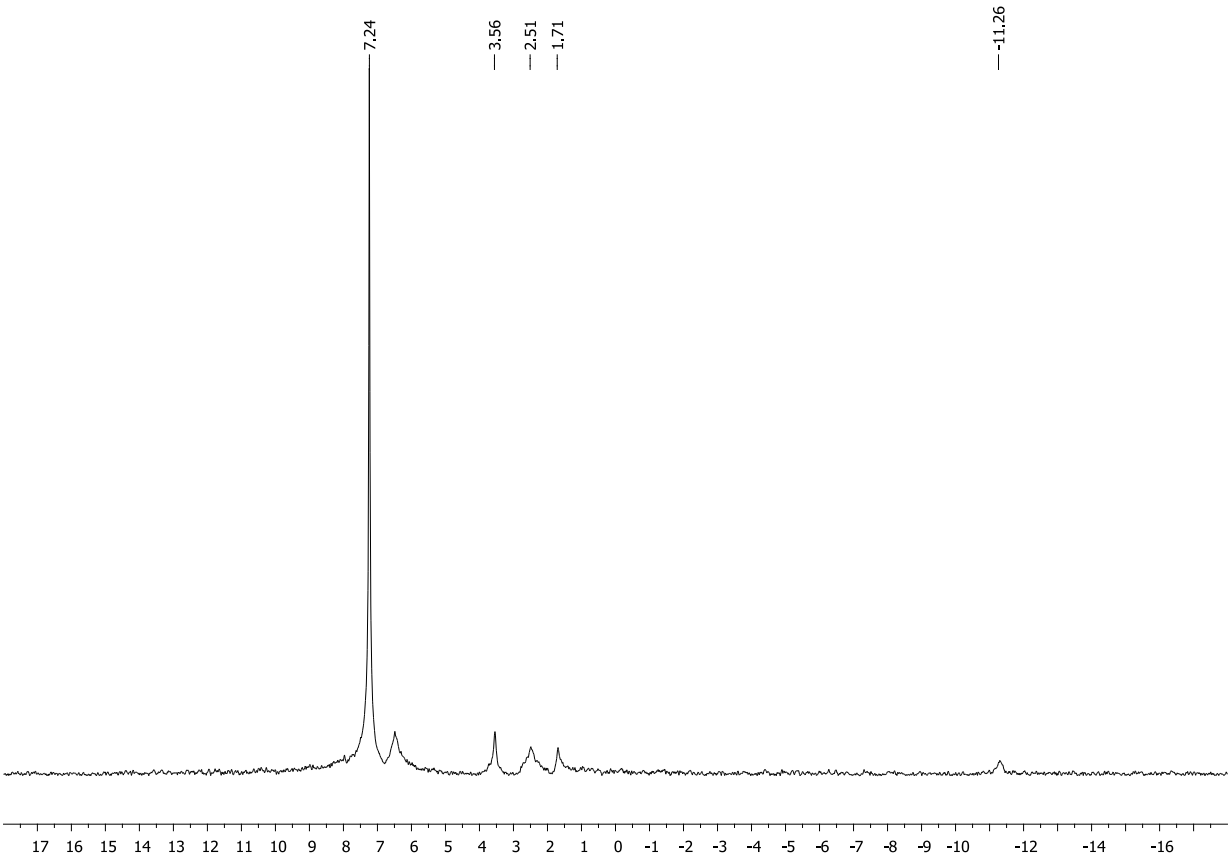


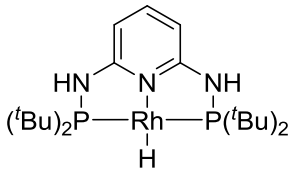
Figure S19 ^{2}D NMR spectrum of **6** with D_2 (THF, 600 MHz, 1000 scan times).

2. Crystallographic data

	2·THF	**4**·0.5C_6H_6	**5**	**5a**·2HCO_2H
Formula	$C_{25}H_{49}ClN_3OP_2Rh$	$C_{30}H_{49}N_3P_2Rh$	$C_{22}H_{41}N_3OP_2Rh$	$C_{25}H_{46}N_3O_7P_2Rh$
Formula weight	607.97	616.57	527.43	665.50
Cryst syst	orthorhombic	monoclinic	orthorhombic	monoclinic
Space group	P 21 21 21	P2(1)/c	P n a 21	P 21
T[K]	173(2)	293(2)	180(2)	200(2)
a[Å]	15.4568(12)	18.9974(2)	22.5273(4)	8.15073(17)
b[Å]	15.5903(8)	8.2894(1)	8.11695(15)	23.7055(6)
c[Å]	16.3952(11)	19.8778(2)	14.1994(2)	8.4853(2)
α[deg]	90	90	90	90
β[deg]	90	91.361(1)	90	100.062(2)
γ[deg]	90	90	90	90
V[Å 3]	3950.9(5)	3129.41(6)	2596.40(8)	1614.28(6)
Z	4	4	4	2
Density[gcm^{-3}]	1.022	1.374	1.352	1.369
F(000)	1280	1360	1108	696
θ range (°)	3.10 to 29.59	2.33 to 76.54	3.92 to 76.26	5.29 to 76.31
Data collected (*hkl*)	$-14\le h\le 19$	$-23\le h\le 23$	$-28\le h\le 26$	$-10\le h\le 10$
	$-19\le k\le 19$	$-6\le k\le 10$	$-10\le k\le 10$	$-29\le k\le 29$
	$-14\le h\le 20$	$-24\le h\le 22$	$-17\le h\le 14$	$-10\le h\le 10$
Reflns collected/ unique	17053/8450	15299/6468	12089/4651	5112/5112
Data/restrains/para	8450/0/298	6468/0/337	4651/1/274	5112/1/328
Goodness-of-fit on F^2	1.055	0.994	1.056	1.016
Final R_1, wR_2 [I>2σ(I)]	0.0625, 0.1171	0.0337, 0.0881	0.0318, 0.0811	0.0464, 0.1100
R_1, wR_2 (all data)	0.0447, 0.1065	0.0300, 0.0797	0.0346, 0.0845	0.0519, 0.1157
Δρmax, min/e Å -3	0.427, –0.696	0.612, –0.540	0.539, –0.670	0.842, –0.703

DFT results:

Aromatized (PN^3P)Rh^IH (**6**)



Sum of electronic and zero-point Energies=	-1781.779586
Sum of electronic and thermal Energies=	-1781.745783
Sum of electronic and thermal Enthalpies=	-1781.744839
Sum of electronic and thermal Free Energies=	-1781.840022

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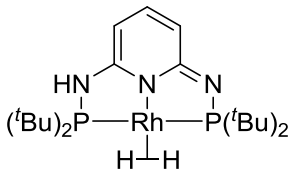
N	0.67097800	0.13107700	-1.22731200
C	1.23245700	-1.02877000	-3.25281200
C	1.27000500	1.38347300	-3.18651500
C	0.87344600	1.31324900	-1.84635800
C	0.84615700	-1.02081800	-1.90823700
H	1.36748900	-1.96942700	-3.77965300
H	1.42810100	2.34727000	-3.66270000
N	0.63240600	-2.18152200	-1.20102200
P	0.02362500	-2.14258200	0.44770300
C	1.26141500	-3.29124900	1.29619800
C	2.49776500	-2.41532600	1.52530200
H	2.90078500	-2.03107400	0.57886200
H	3.28171400	-3.01207600	2.01441400
H	2.25881000	-1.55147400	2.15831900
C	0.70392300	-3.71767700	2.65260300
H	1.50249300	-4.19322700	3.23940900
H	-0.10906000	-4.44838400	2.55686500
H	0.33578000	-2.85613600	3.22530900
C	1.67904700	-4.51860400	0.48906300
H	2.15353000	-4.23687700	-0.45893600
H	0.84966100	-5.20182900	0.27768100
H	2.42709800	-5.08520800	1.06184900
C	-1.67109400	-2.96735800	0.25928800
C	-2.42580600	-2.79905000	1.57988000
H	-1.98532900	-3.38498700	2.39411600
H	-3.46273000	-3.14093600	1.44982700
H	-2.43944700	-1.74716300	1.89097000

C	-2.40214900	-2.15297200	-0.81259600
H	-1.95874000	-2.28422100	-1.80735800
H	-2.38960500	-1.08062200	-0.57326000
H	-3.44897400	-2.48443000	-0.86312200
C	-1.65716600	-4.43525300	-0.15242800
H	-1.09586000	-4.60520900	-1.08118500
H	-2.68813100	-4.77060800	-0.33724000
H	-1.24273300	-5.08471200	0.62772200
N	0.65930500	2.43817200	-1.08471800
P	0.22659100	2.32528900	0.61549400
C	1.69395200	3.19918100	1.43118800
C	-1.33400300	3.39293600	0.64028800
C	-1.27691300	4.67428400	-0.18887900
C	-2.42365300	2.48703700	0.05751400
C	-1.69471200	3.72276700	2.08771500
C	1.89987200	4.65997400	1.04563400
C	2.92118700	2.38856000	1.00092800
C	1.54896000	3.06845700	2.94823200
H	-2.54735400	1.57869100	0.66057600
H	-3.37706600	3.03511500	0.03449100
H	-2.18382000	2.17558500	-0.96769400
H	-1.03301300	4.48501900	2.51726900
H	-2.71797500	4.12257200	2.12420100
H	-1.66085200	2.82977900	2.72574900
H	-1.09631200	4.46698800	-1.25101300
H	-2.25061100	5.18100100	-0.12763000
H	-0.52170300	5.38412800	0.16323200
H	2.86023300	5.01152600	1.44995600
H	1.94008500	4.80480300	-0.04270300
H	1.12172700	5.31595400	1.45318100
H	2.78932900	1.32098900	1.22680400
H	3.12399300	2.48594100	-0.07259700
H	3.80232700	2.75407700	1.54712500
H	2.47089400	3.42269400	3.43136200
H	0.71958400	3.66414600	3.34495400
H	1.38434600	2.02296600	3.23642600
H	0.84835800	3.32195200	-1.54109900
Rh	0.05832900	0.08178600	0.82444400
H	0.70428400	-3.03823000	-1.73618800
H	-0.41496300	0.03336600	2.37225500

Dearomatized (PN^3P)$Rh^I(H_2)$ (**6a**)

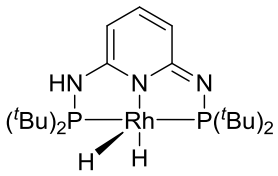


Sum of electronic and zero-point Energies= -1781.773782
Sum of electronic and thermal Energies= -1781.739279
Sum of electronic and thermal Enthalpies= -1781.738335
Sum of electronic and thermal Free Energies= -1781.836077

H	1.97302400	0.17397700	-4.82897600
C	1.59188800	0.15132000	-3.80948700
N	0.63077700	0.11157900	-1.21011300
C	1.33590000	-1.05167900	-3.20842000
C	1.36830400	1.36063300	-3.13463500
C	0.87865900	1.28713900	-1.84205200
C	0.83984400	-1.10381500	-1.87220300
H	1.49764000	-1.99918900	-3.71163500
H	1.55507800	2.32452200	-3.59936900
N	0.59708700	-2.26689200	-1.29272100
P	0.00687600	-2.19214100	0.27050100
C	1.24038700	-3.23308200	1.24666900
C	2.48600400	-2.34549300	1.35349900
H	2.84633800	-2.04504400	0.36133000
H	3.29030300	-2.90397400	1.85390200
H	2.28516000	-1.43305800	1.93116000
C	0.73831000	-3.55431000	2.65059100
H	1.55652400	-3.99520700	3.23816100
H	-0.08107700	-4.28329200	2.64177000
H	0.39685300	-2.65618400	3.18399700
C	1.62640200	-4.51630000	0.51292700
H	1.91872300	-4.30204300	-0.52029000
H	0.81264500	-5.24834800	0.49341700
H	2.47713200	-4.98444800	1.02935100
C	-1.69734100	-2.99281300	0.17274900
C	-2.44494500	-2.84882600	1.49668200
H	-1.96329200	-3.39073400	2.31822100
H	-3.46085300	-3.25510700	1.38631800
H	-2.53576600	-1.79499700	1.78957100
C	-2.44584800	-2.19320800	-0.89841500
H	-1.97479700	-2.30409000	-1.88133100
H	-2.47954900	-1.12197300	-0.65359700

H	-3.47990800	-2.56088100	-0.96548000
C	-1.64620700	-4.45705600	-0.25399000
H	-1.02146200	-4.59100900	-1.14504800
H	-2.66257000	-4.80075300	-0.49600200
H	-1.26690600	-5.10820000	0.54298100
N	0.60261900	2.44154700	-1.11995400
P	0.17468800	2.36272900	0.54651900
C	1.64869300	3.15980200	1.41980700
C	-1.36079100	3.45582600	0.59421500
C	-1.25463000	4.73823800	-0.22926700
C	-2.47228500	2.58646100	-0.00309300
C	-1.71190600	3.79081300	2.04199300
C	1.83476400	4.65214500	1.16667000
C	2.87642100	2.40243300	0.90262700
C	1.52198200	2.89964000	2.92219400
H	-2.65925100	1.69437000	0.60749400
H	-3.40086900	3.17221500	-0.06010400
H	-2.21841900	2.24710800	-1.01548200
H	-1.01262900	4.51166800	2.48355200
H	-2.71265300	4.24313700	2.07870400
H	-1.73330700	2.89391800	2.67621700
H	-1.08652100	4.52407600	-1.29147900
H	-2.20613700	5.28418600	-0.16277200
H	-0.46768200	5.41289600	0.12251400
H	2.78661200	4.97877900	1.60942500
H	1.88017900	4.89544700	0.09683200
H	1.04164900	5.25378400	1.62629200
H	2.75077900	1.31505400	1.00039400
H	3.08300900	2.62222000	-0.15148000
H	3.75556100	2.70086300	1.49048500
H	2.41664700	3.28339300	3.43236100
H	0.65188000	3.39528000	3.36798100
H	1.45014300	1.82485500	3.13083000
H	0.83767100	3.31061700	-1.58312500
Rh	-0.03606600	0.06998300	0.75784300
H	-0.96127400	0.05967900	2.18311600
H	-0.15959800	-0.16655600	2.43530300

Dearomatized (PN^3P)$Rh^{III}H_2$ (**6b**)

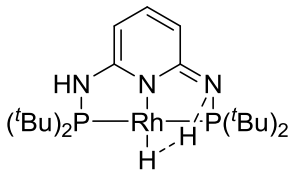


Sum of electronic and zero-point Energies= -1781.745595
Sum of electronic and thermal Energies= -1781.712286
Sum of electronic and thermal Enthalpies= -1781.711342
Sum of electronic and thermal Free Energies= -1781.805151

H	-0.42657700	0.38205700	-5.24017400
C	-0.29880700	0.28274100	-4.16137800
N	-0.02768700	0.09338200	-1.45701900
C	-1.09168800	-0.60075500	-3.47541700
C	0.69435200	1.05223500	-3.52393500
C	0.79721800	0.89286100	-2.14690000
C	-0.96651000	-0.71978700	-2.06114100
H	-1.85730300	-1.19090400	-3.96898900
H	1.35743800	1.71165800	-4.06600000
N	-1.73826500	-1.53957100	-1.34575400
P	-1.96550400	-1.13753200	0.26447600
C	-2.42921600	-2.76379100	1.07944300
C	-1.11351700	-3.53034000	1.26287000
H	-0.61595900	-3.70886500	0.30477600
H	-1.34029700	-4.50841200	1.71694400
H	-0.42755300	-2.99750900	1.92670700
C	-3.06409900	-2.55871700	2.44863800
H	-3.15754200	-3.52964100	2.95089200
H	-4.07148200	-2.12655200	2.38312000
H	-2.44681300	-1.90751000	3.09287500
C	-3.34181600	-3.59415200	0.18757600
H	-2.92011100	-3.70222300	-0.81607300
H	-4.34249400	-3.16794200	0.09634700
H	-3.45023300	-4.59761700	0.62325600
C	-3.44912000	0.07189100	0.27833600
C	-3.69327700	0.67456700	1.66729200
H	-4.02105000	-0.06609600	2.40218700
H	-4.47397300	1.44725000	1.58907700
H	-2.78047300	1.15791500	2.05687500
C	-3.07954000	1.21684200	-0.67212200

H	-2.94346400	0.87336700	-1.70856000
H	-2.15743000	1.73012800	-0.36413300
H	-3.88757700	1.96243000	-0.67086100
C	-4.73326800	-0.57634400	-0.23845100
H	-4.56619700	-1.09406500	-1.19983600
H	-5.49821700	0.19914900	-0.41140100
H	-5.16257700	-1.29683200	0.46888100
N	1.77362700	1.53946700	-1.38036800
P	2.04678900	1.02508200	0.25590100
C	3.63617600	0.00791600	0.18899200
C	2.31462200	2.69077100	1.10410000
C	3.22142500	3.65959100	0.34314800
C	0.90780600	3.30629300	1.21978800
C	2.86474900	2.44636700	2.51416500
C	4.89477400	0.79189400	-0.17998400
C	3.38165400	-1.05766900	-0.89240700
C	3.82070500	-0.69218200	1.52780800
H	0.24533400	2.70089800	1.85601500
H	0.98119900	4.31851500	1.66295300
H	0.44153100	3.41791300	0.22179800
H	3.91305000	2.11914400	2.49861600
H	2.82756800	3.39226900	3.08586000
H	2.26558600	1.69892400	3.05270200
H	2.80290300	3.91886900	-0.63524000
H	3.30393600	4.60441000	0.91134200
H	4.24622300	3.27544700	0.19946100
H	5.72496600	0.08294600	-0.31898800
H	4.78613300	1.34843500	-1.11396900
H	5.19766100	1.49240100	0.61670900
H	2.45634400	-1.62148400	-0.69597100
H	3.29713900	-0.61808000	-1.89492600
H	4.21738100	-1.76064600	-0.89534900
H	4.67026400	-1.40013600	1.45545400
H	4.05798100	0.00848900	2.33859700
H	2.92881300	-1.25435900	1.81135000
H	2.48368200	2.03451700	-1.90705500
Rh	0.03558100	-0.10980500	0.66129600
H	0.63693300	-1.52062000	0.77473000
H	0.07889000	-0.33521700	2.24437000

Transition State (**6TS**)



Sum of electronic and zero-point Energies= -1781.697965
Sum of electronic and thermal Energies= -1781.664618
Sum of electronic and thermal Enthalpies= -1781.663674
Sum of electronic and thermal Free Energies= -1781.758181

H	-0.27008100	0.26405500	0.13340200
C	-0.16084200	0.18828600	1.21352700
N	0.09551400	0.03299400	3.91900500
C	-0.99728400	-0.66458300	1.92321900
C	0.83764900	0.92667500	1.84422100
C	0.94580700	0.80284400	3.23171100
C	-0.83535200	-0.75669000	3.31099600
H	-1.74942200	-1.27456800	1.43416000
H	1.52404400	1.55688000	1.28521300
N	-1.48621700	-1.67254600	4.10421800
P	-1.87630000	-1.15222100	5.72100200
C	-2.34432700	-2.81166200	6.47957700
C	-1.04268900	-3.60058200	6.65492200
H	-0.57992500	-3.83860400	5.68993200
H	-1.27350700	-4.55128800	7.15641500
H	-0.31462900	-3.05078700	7.26306100
C	-2.95671900	-2.59077800	7.86073000
H	-3.07093700	-3.56233200	8.36088300
H	-3.95326100	-2.13581300	7.80775000
H	-2.31492800	-1.96247500	8.49289200
C	-3.28527400	-3.63198600	5.59694000
H	-2.88353800	-3.73168300	4.58330400
H	-4.28903300	-3.20221100	5.52873400
H	-3.38872200	-4.63616300	6.03179400
C	-3.35212500	0.03419300	5.67235500
C	-3.52143100	0.66861800	7.05419000
H	-3.83141000	-0.04972100	7.82027400
H	-4.29652100	1.44651800	6.99734700
H	-2.58944500	1.14114100	7.39138400
C	-2.98402600	1.14696000	4.68712600
H	-2.90708000	0.77972200	3.65650100
H	-2.03285400	1.62571900	4.95417000

H	-3.77244700	1.91242000	4.71157800
C	-4.64968800	-0.61693400	5.20744200
H	-4.51452600	-1.14660100	4.25561800
H	-5.40932200	0.16292900	5.05097800
H	-5.05473600	-1.31951200	5.94489900
N	1.92805600	1.41294300	3.99464100
P	2.18160600	0.89016100	5.64817500
C	3.82406200	-0.03676100	5.56907000
C	2.34117400	2.55324000	6.51511300
C	3.16288700	3.59860900	5.76358800
C	0.90016000	3.06098900	6.63677000
C	2.91377100	2.33702000	7.91434800
C	5.04392700	0.80431400	5.21085400
C	3.61713500	-1.11556400	4.50144300
C	4.03926400	-0.72931400	6.91716100
H	0.28269600	2.37813900	7.23639000
H	0.90114900	4.04619500	7.12511700
H	0.42910700	3.16926100	5.65111500
H	3.98177500	2.08779500	7.88856900
H	2.80771000	3.26317000	8.49597600
H	2.38199400	1.54093100	8.45224100
H	2.72322800	3.83319800	4.78676600
H	3.16806700	4.53214500	6.34382300
H	4.20716500	3.30311400	5.61740100
H	5.91405200	0.14467300	5.08276500
H	4.91751400	1.35157200	4.26672100
H	5.29699800	1.52487200	5.99745000
H	2.72373900	-1.71829600	4.71262600
H	3.51004500	-0.68859800	3.49654600
H	4.48802400	-1.78526700	4.49277200
H	4.90978900	-1.39632100	6.84379800
H	4.23507000	-0.01973800	7.72927900
H	3.16593000	-1.33144500	7.19710600
H	2.63900300	1.91565000	3.47679400
Rh	0.18638700	-0.25450100	6.03307400
H	-0.28060600	-1.66334100	5.01862100
H	0.26815500	-0.53836800	7.62627200