Supporting Information for

Synthesis and Characterization of Rhodium-Aluminum Heterobimetallic Complexes Tethered by a 1,3-Bis(diphenylamino)-2-propanoxy Group

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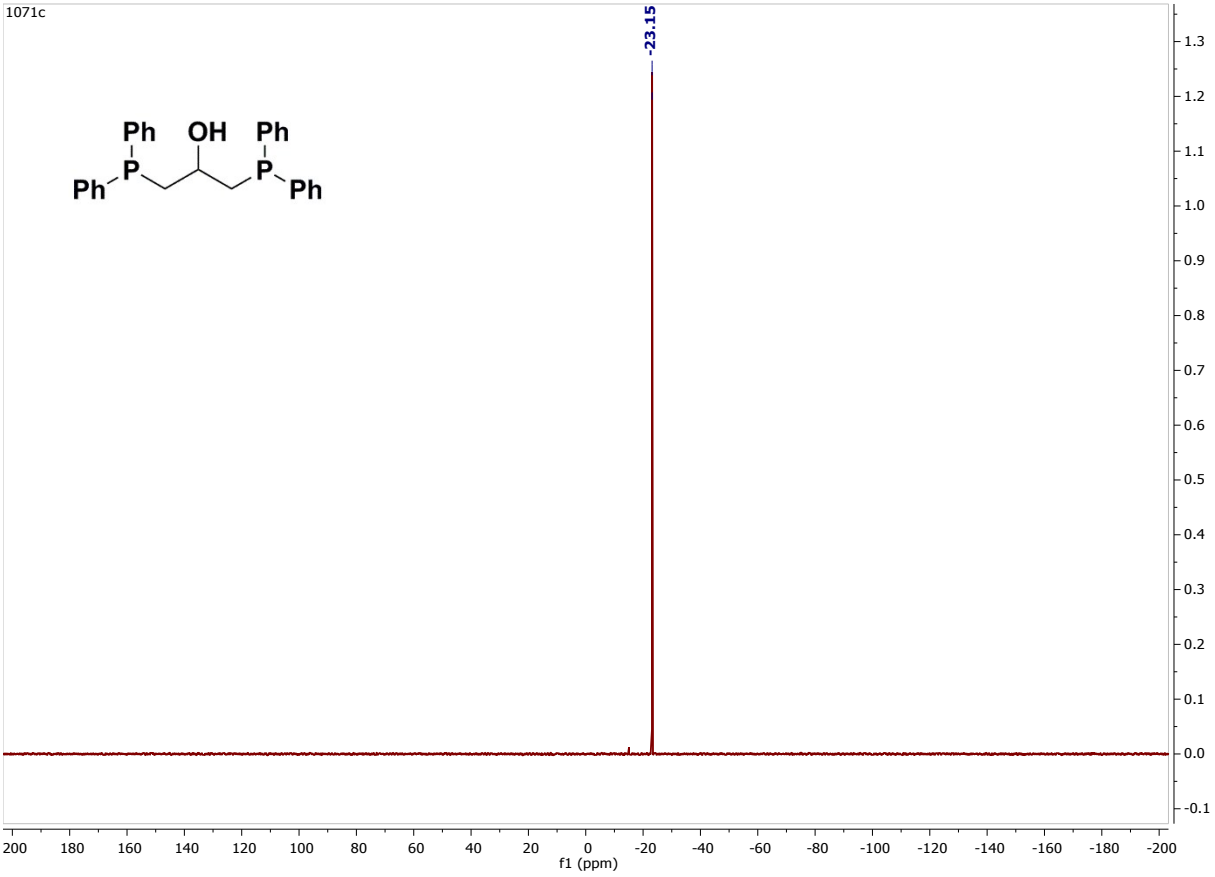


Figure S1. $^{31}P\{^{1}H\}$ NMR spectrum of DPPP-OH in $CDCl_3$.

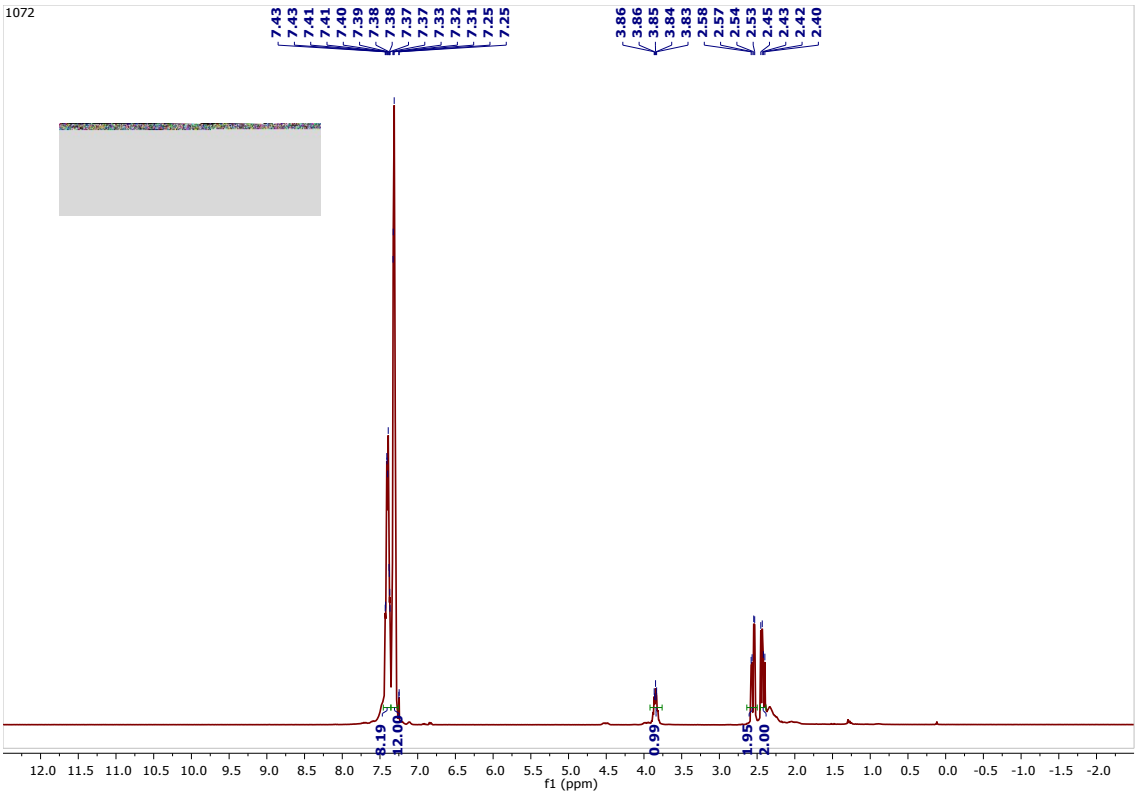


Figure S2. ^{1}H NMR spectrum of DPPP-OH in $CDCl_3$.

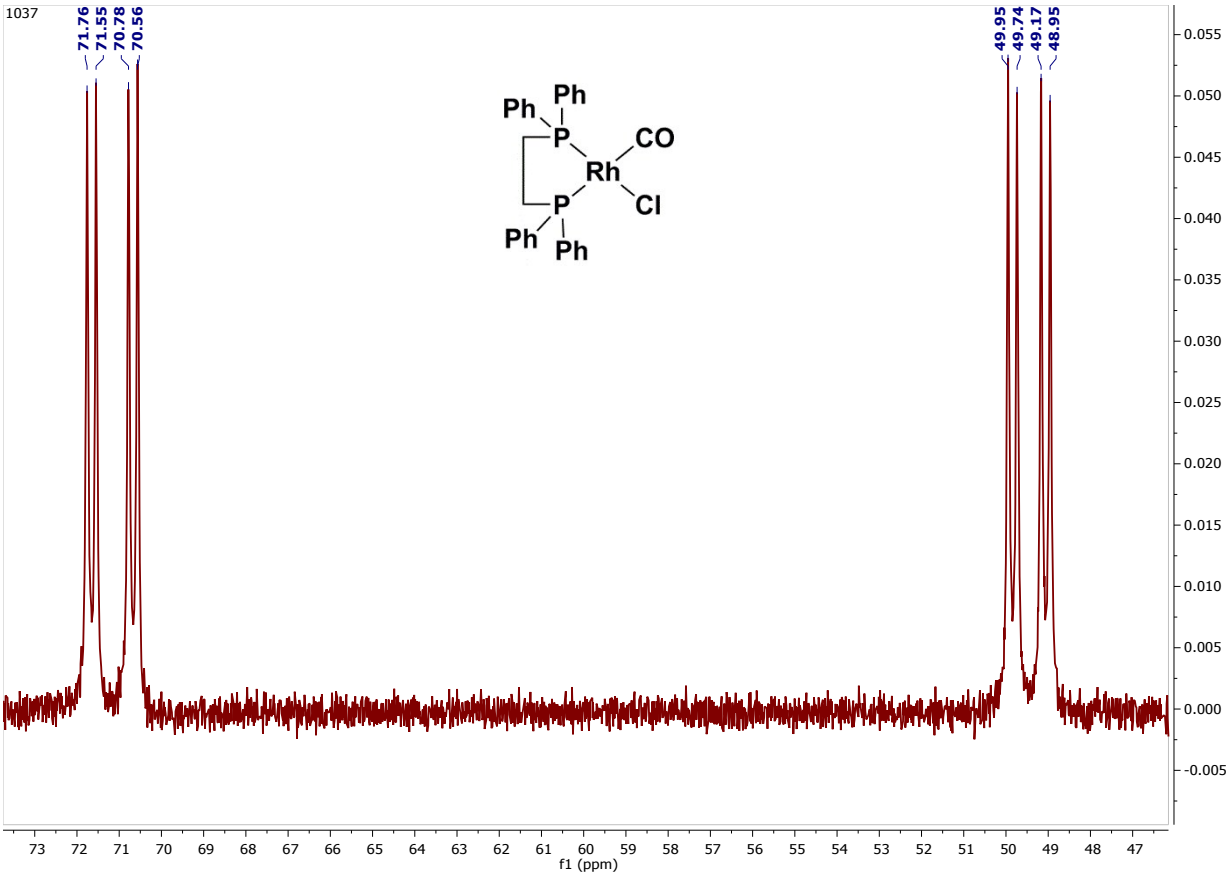


Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum of Rh(DPPE)(CO)Cl in $CDCl_3$.

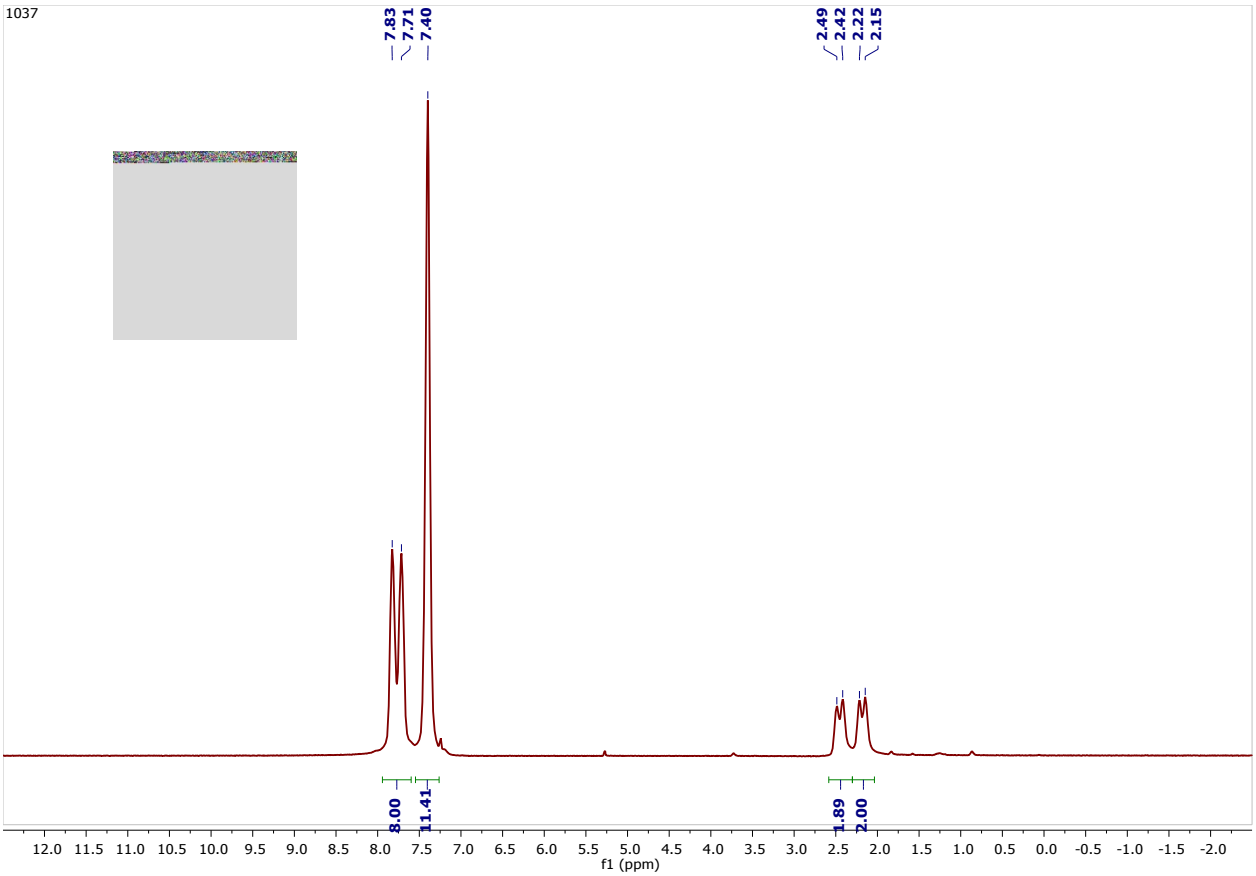


Figure S4. ^{1}H NMR spectrum of Rh(DPPE)(CO)Cl in $CDCl_3$.

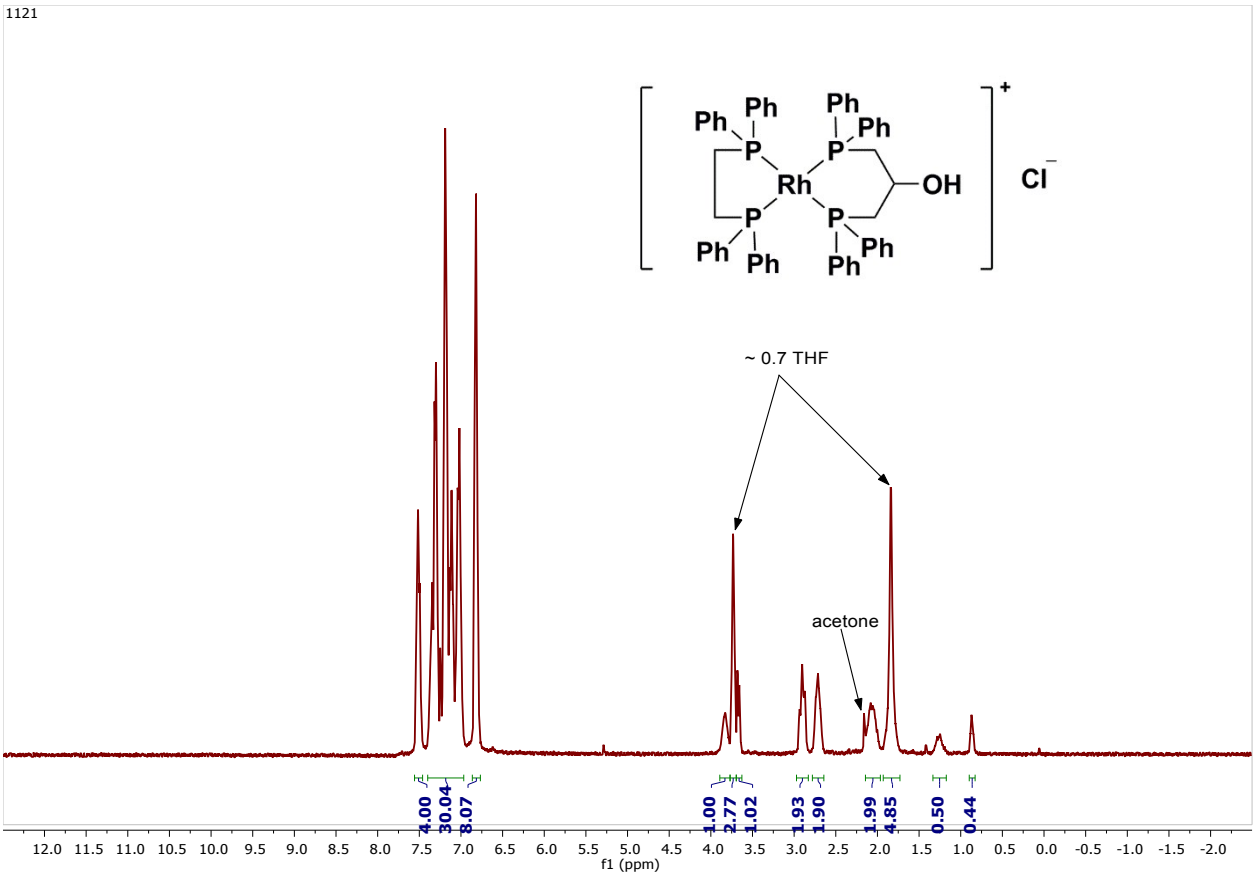


Figure S5. ^{1}H NMR spectrum of Rh(DPPE)(DPPP-OH)Cl (**1**) in $CDCl_3$.

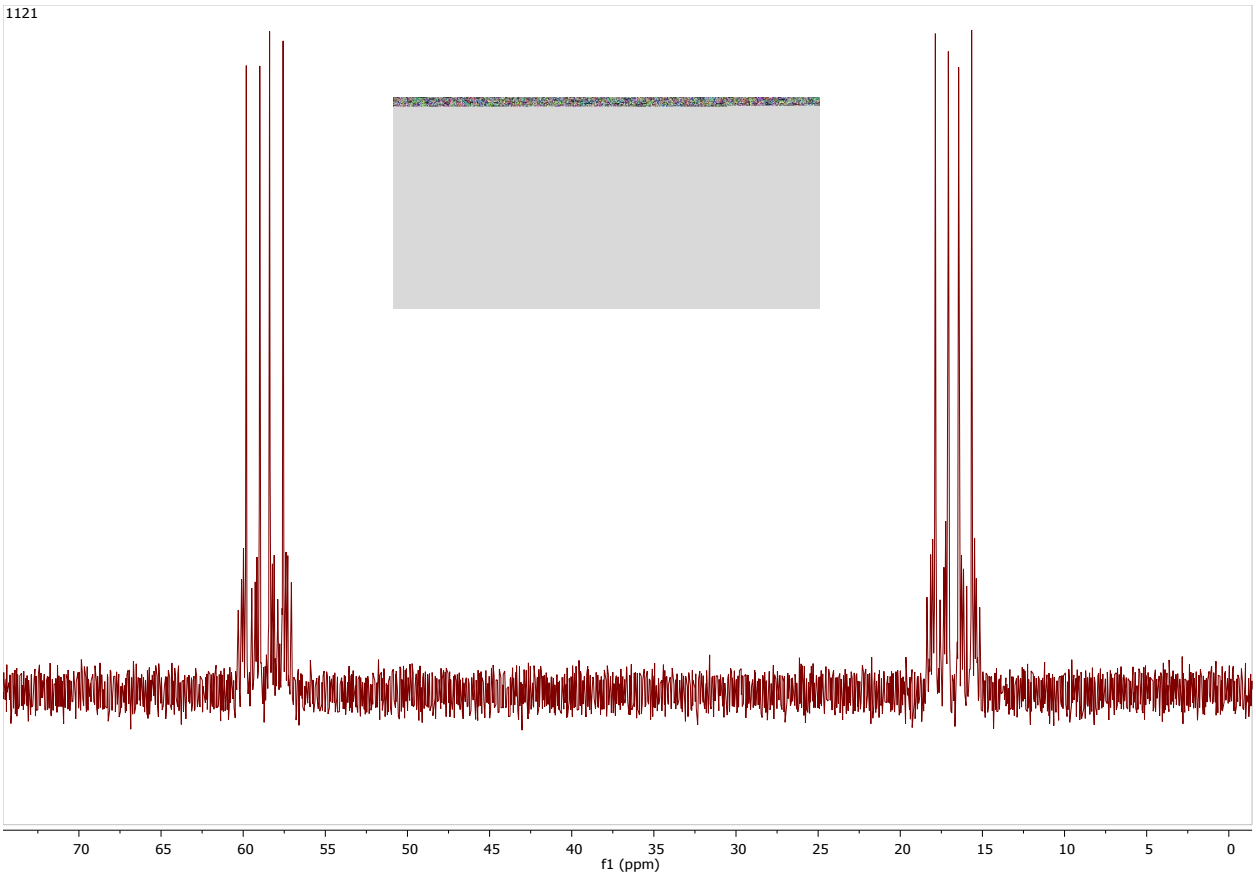


Figure S6. $^{31}P\{^{1}H\}$ NMR spectrum of **1** in $CDCl_3$.

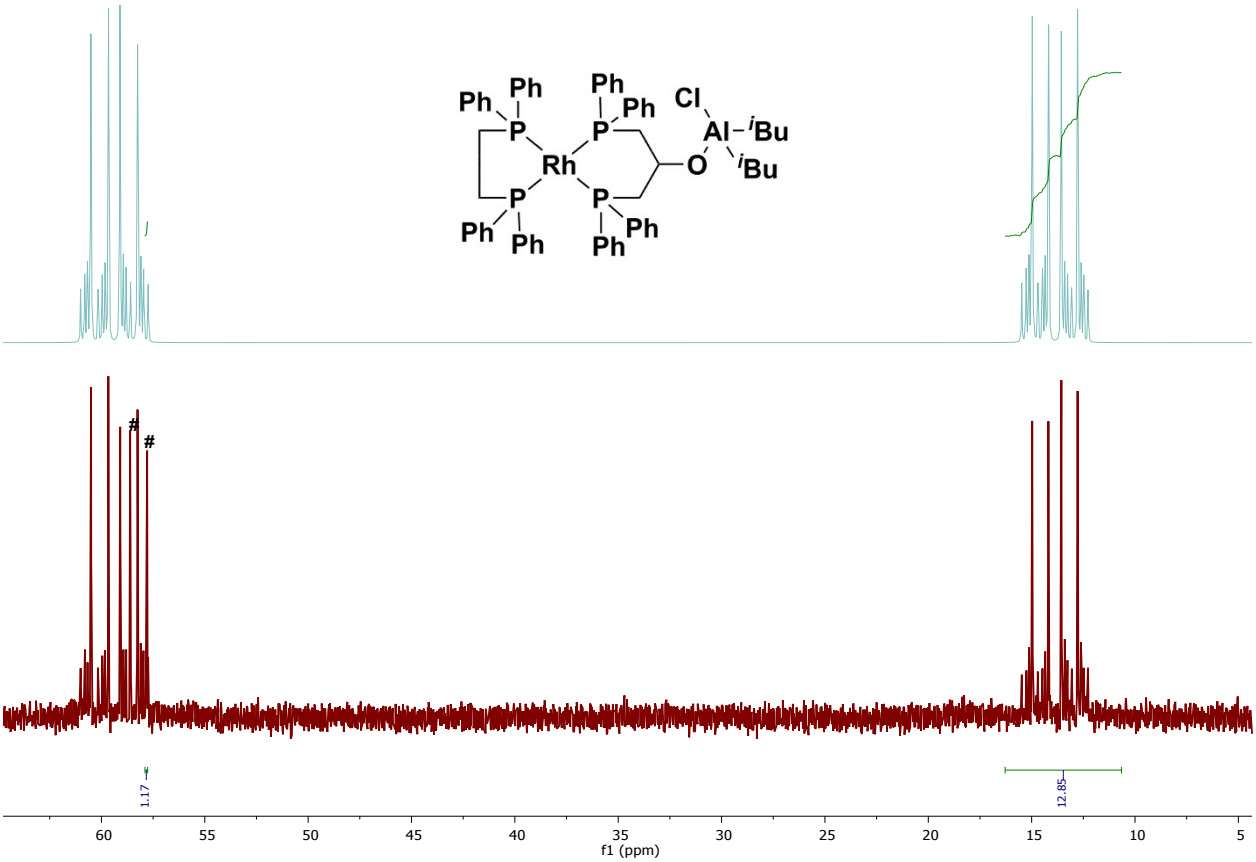


Figure S7. Modeled (top) and measured (bottom) $^{31}P\{^{1}H\}$ NMR spectra of Rh(DPPE)(DPPP-O-Al^{i}Bu$_2$Cl) (**2**). The peaks for byproduct Rh(DPPE)$_2$Cl are denoted with #. Integration values used to quantify byproduct.

List of peaks and coupling constants in **2**: $^{31}P\{^{1}H\}$ NMR (162 MHz, THF-d$_8$) δ 59.37 (DP*P*E, J_{Rh} = 107.2 Hz, J_{trans} = 205.5 Hz, $J_{cis,\ B\text{-}B'}$ = -22.6 Hz, $J_{cis,\ B\text{-}A'}$ = -29.2 Hz), 58.20 (Rh(DP*P*E)$_2$Cl, d, J = 132.8 Hz), 13.90 (DP*P*P-OH, *ddd*, J_{Rh} = 101.2 Hz, J_{trans} = 205.5 Hz, $J_{cis\ A\text{-}A'}$ = -39.4 Hz, $J_{cis,\ A\text{-}B'}$ = -29.2 Hz).

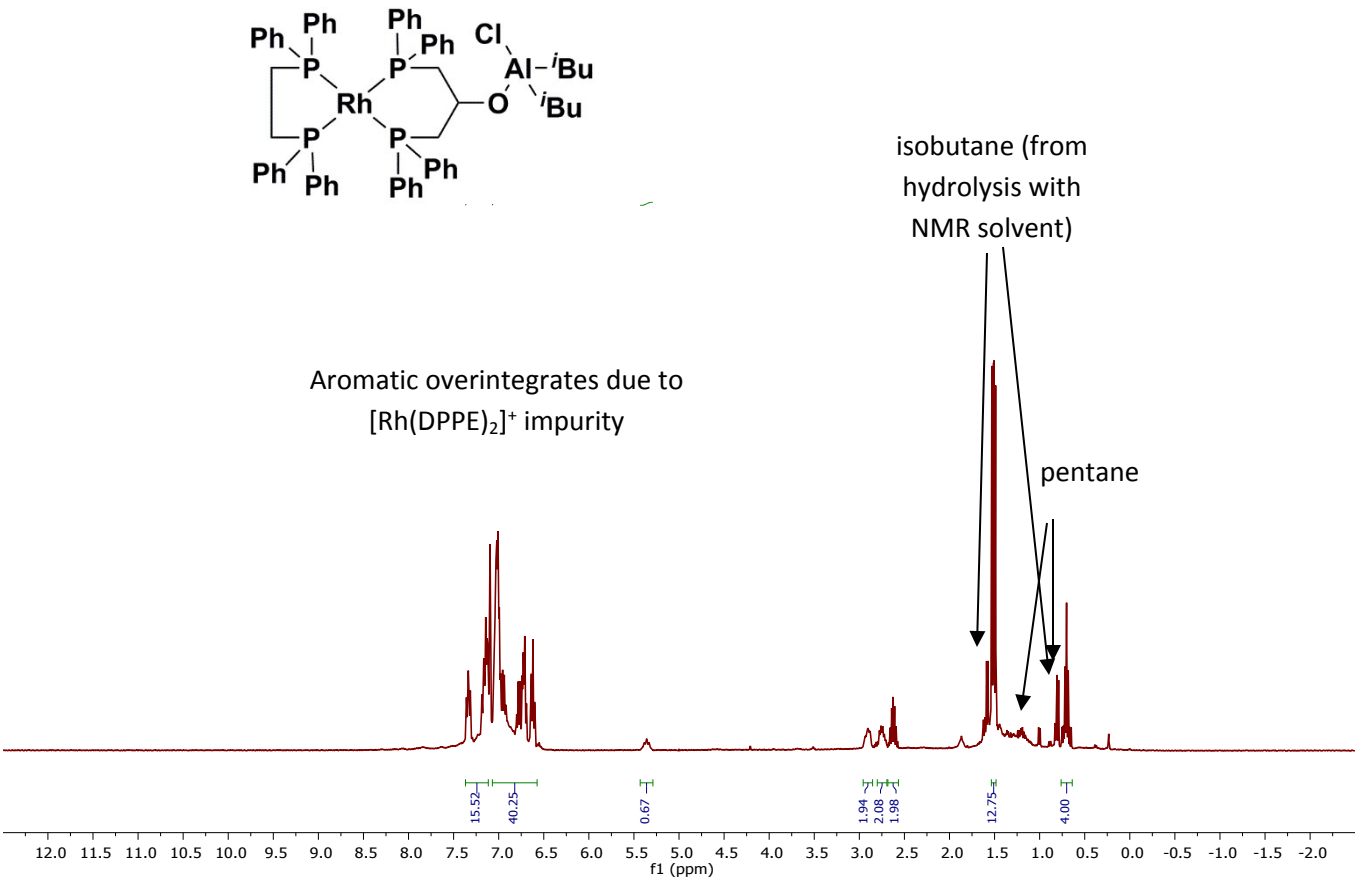


Figure S8. ^{1}H NMR spectrum of **2**. Impurity in alkyl region is pentane. Overintegration of aromatic signals due to 5% $[Rh(DPPE)_2]Cl$ impurity.

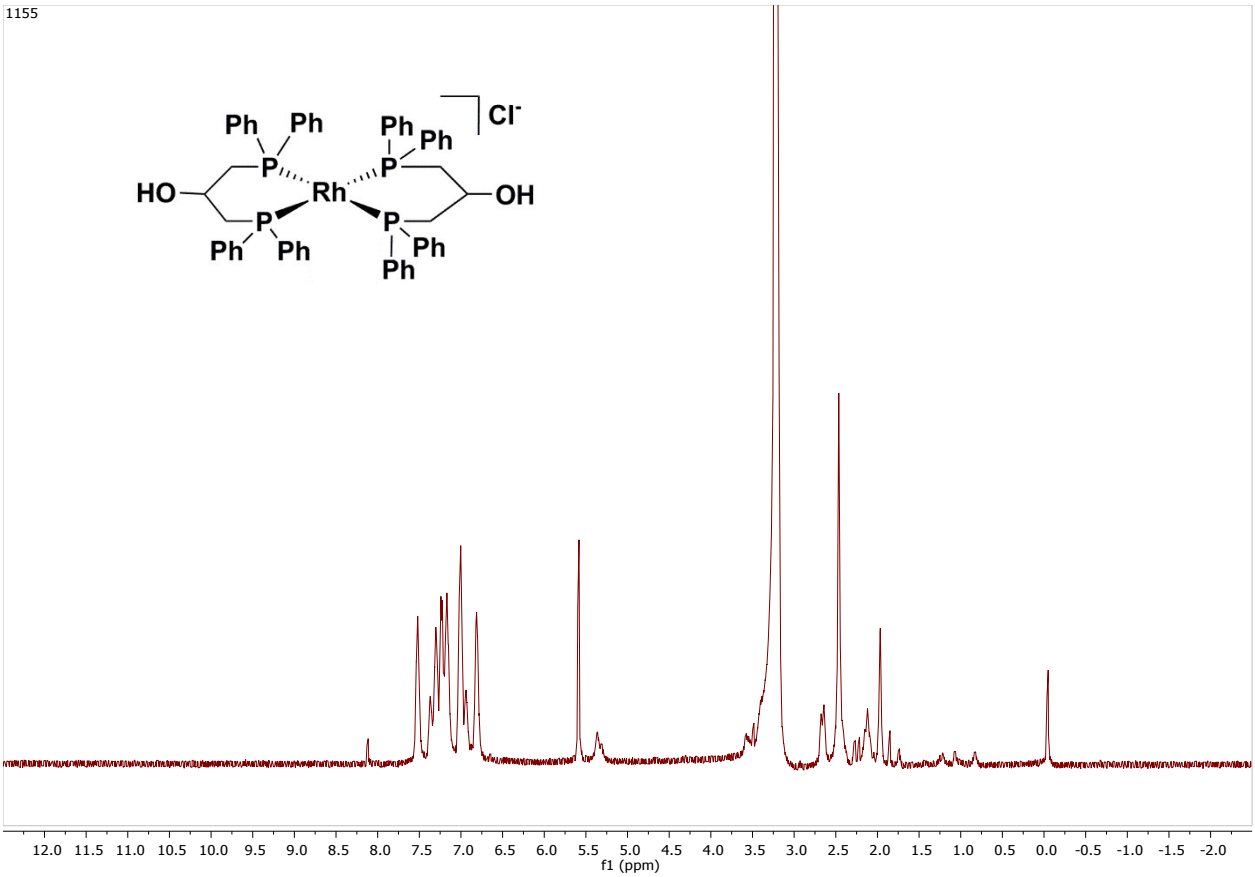


Figure S9. ^{1}H NMR spectrum of isomeric mixture of Rh(DPPP-OH)$_2$Cl (**3**) in DMSO-d_6.

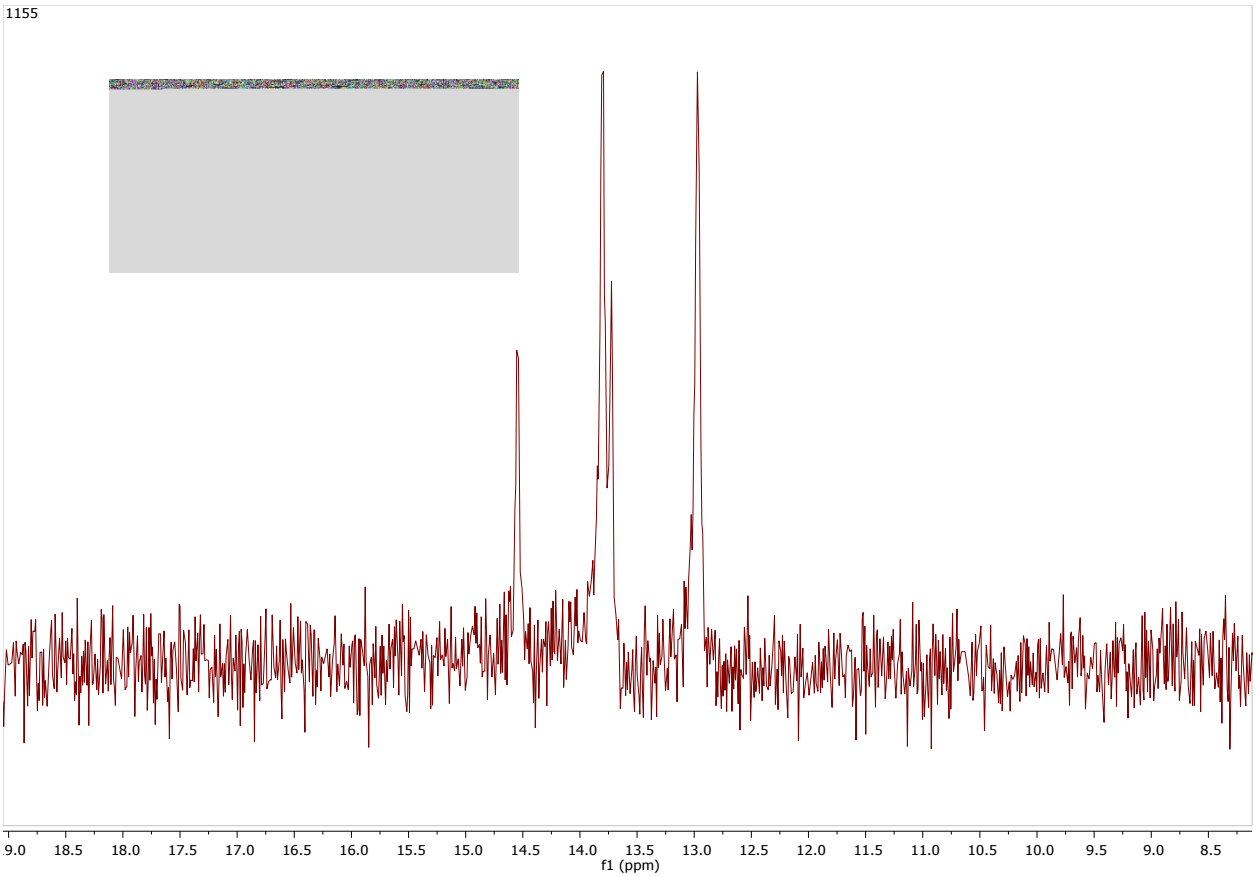


Figure S10. $^{31}P\{^{1}H\}$ NMR spectrum of isomeric mixture **3** in DMSO-d_6.

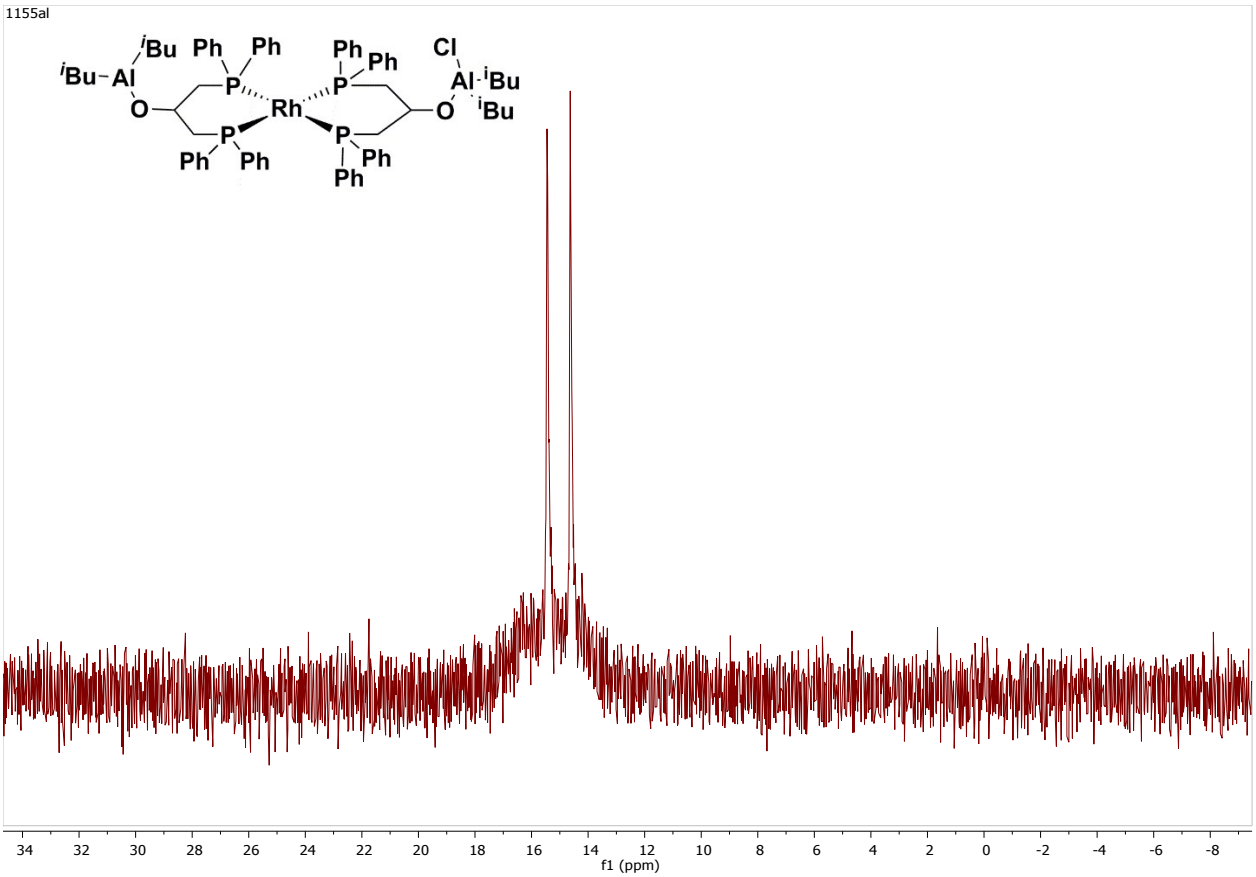


Figure S11. Room temperature $^{31}P\{^{1}H\}$ NMR spectrum of Rh(DPPP-O-Al^{i}Bu$_2$)(DPPP-O-Al^{i}Bu$_2$Cl) (**4**) in CD_2Cl_2.

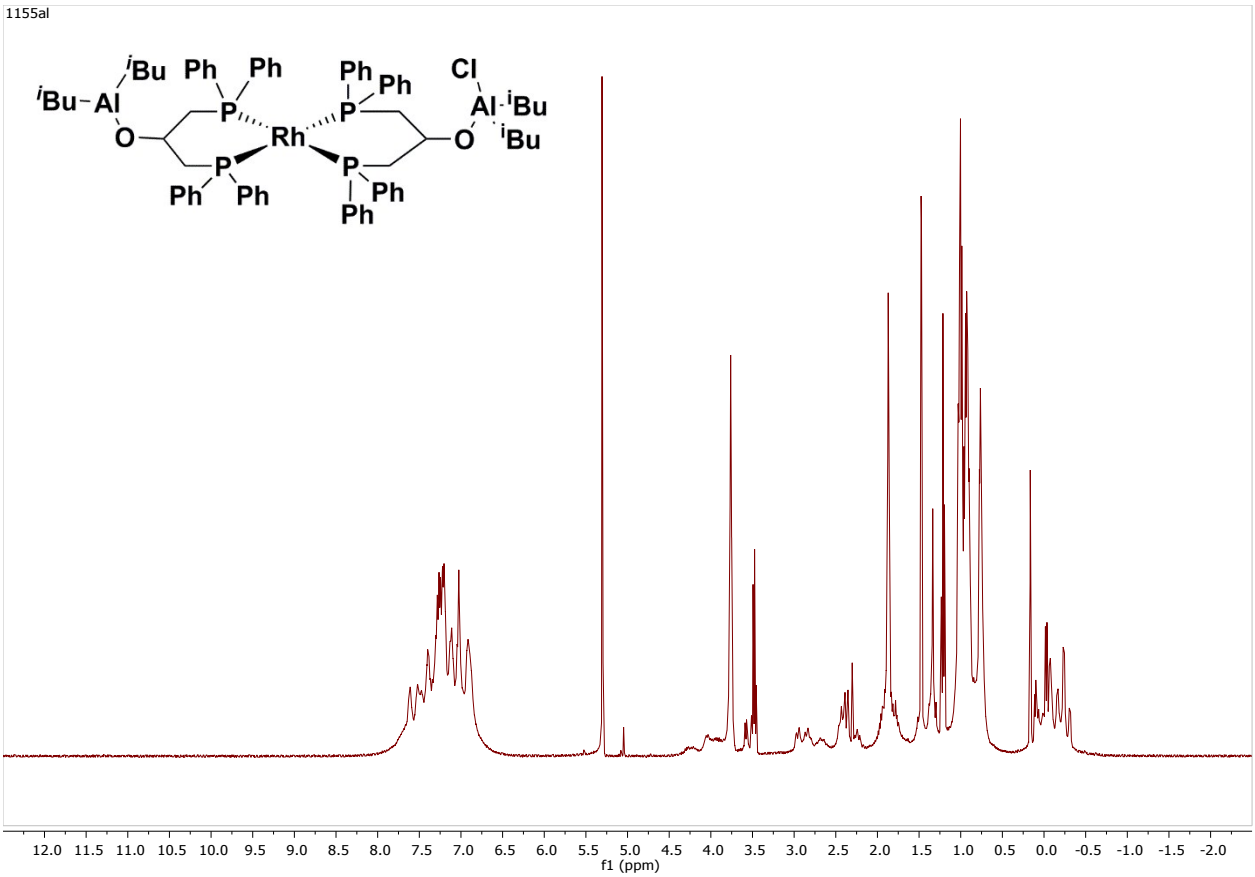
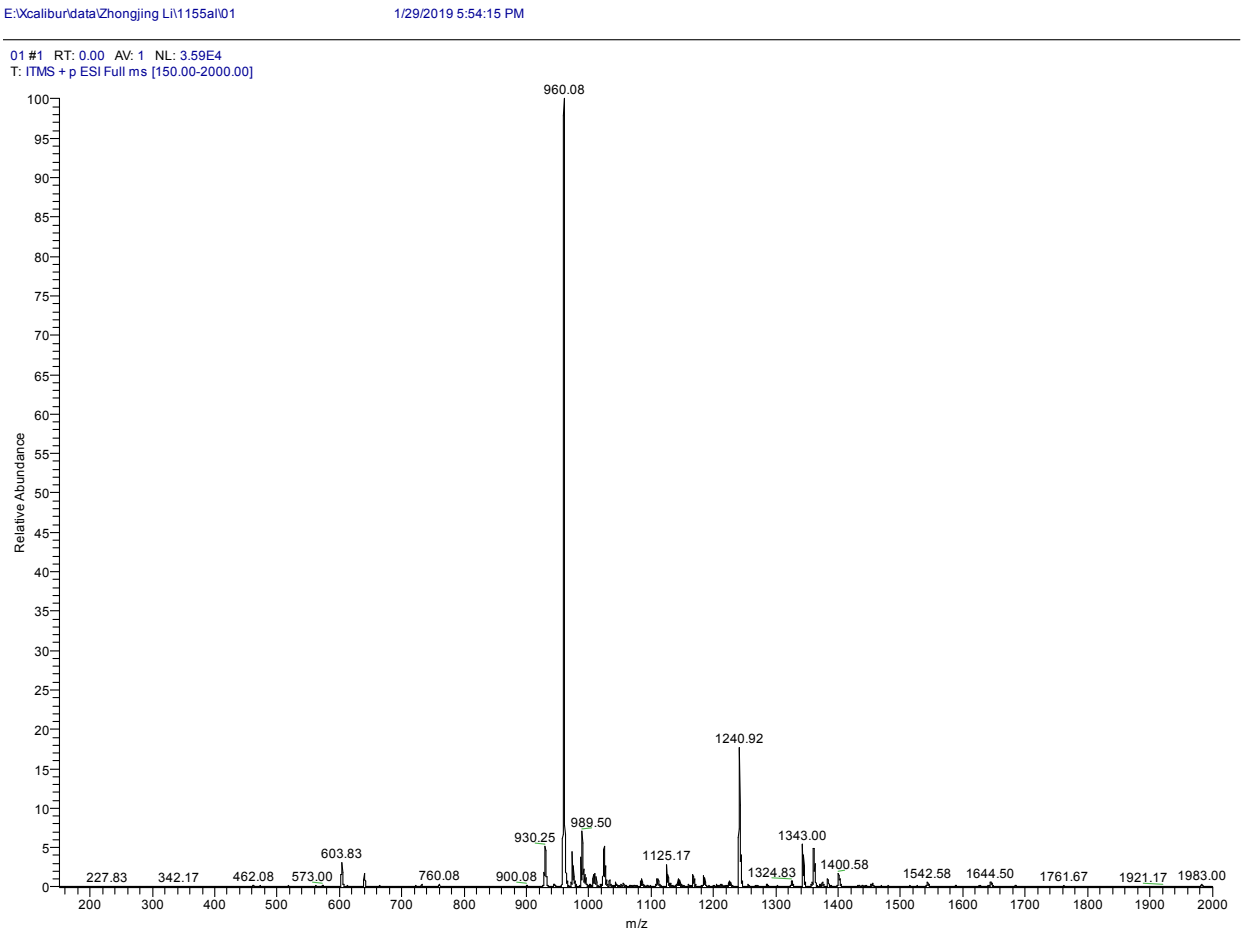
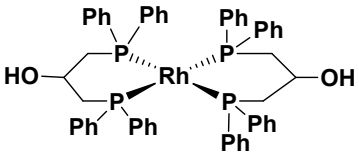


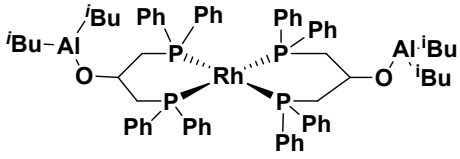
Figure S12. ^{1}H NMR of **4** product mixture in CD_2Cl_2.





A

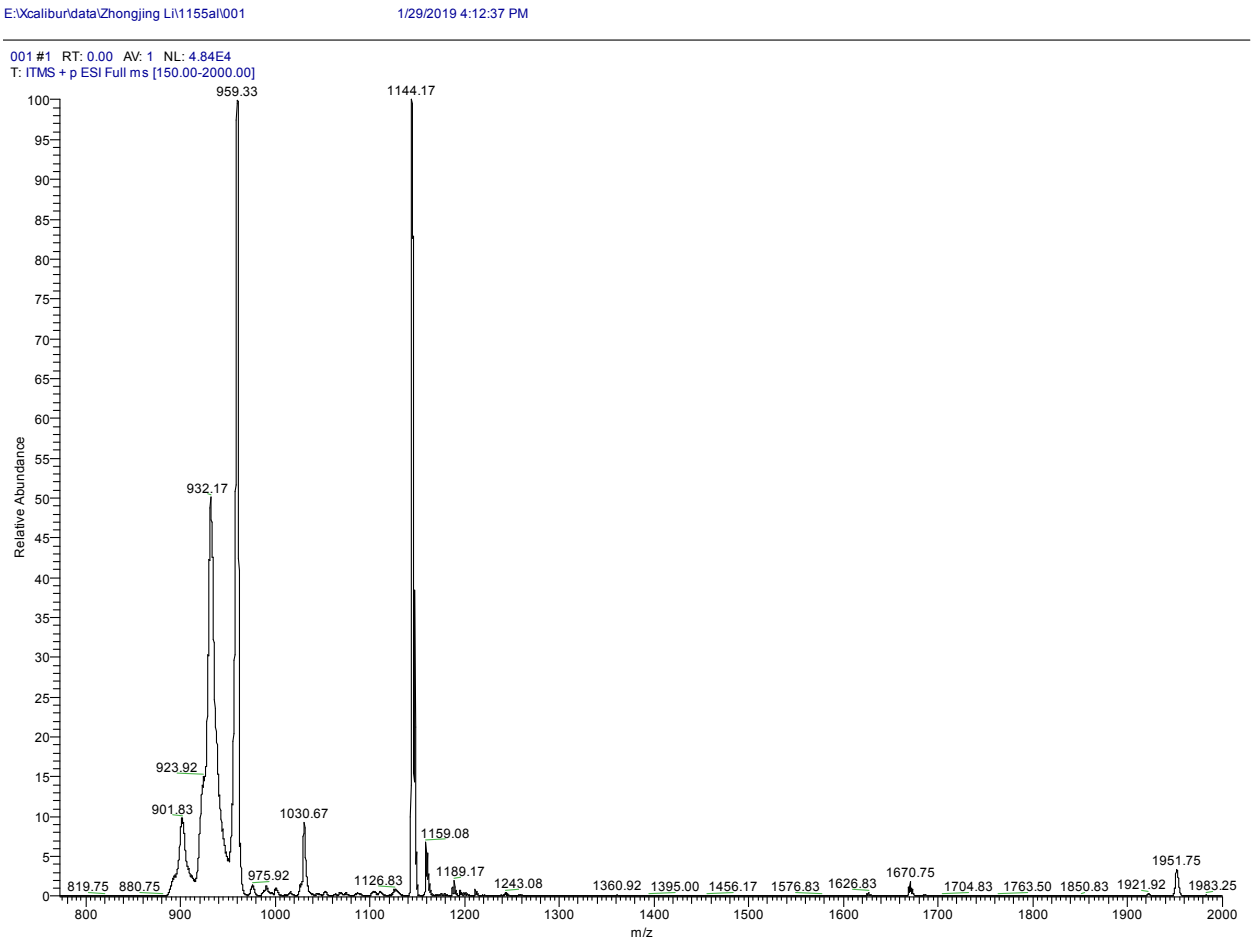
Chemical Formula: $C_{54}H_{52}O_2P_4Rh$
Exact Mass: 959.20
Molecular Weight: 959.81
m/z: 959.20 (100.0%), 960.20 (58.4%), 961.20 (16.7%), 962.21 (2.3%)

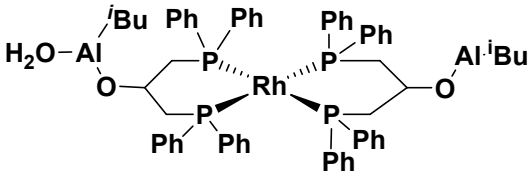


B

Chemical Formula: $C_{70}H_{86}Al_2O_2P_4Rh$
Exact Mass: 1239.43
Molecular Weight: 1240.22
m/z: 1239.43 (100.0%), 1240.43 (75.7%), 1241.43 (28.3%), 1242.44 (6.7%), 1243.44 (1.3%)

Figure S13. ESI-MS data for **4**. The base peak (m/z = 960 corresponds to fragment A above. The high mass peak (m/z =1240) corresponds to fragment B above. Isotope pattern from high-resolution experiment can be found in Figure S15, below.





Chemical Formula: $C_{62}H_{70}Al_2O_3P_4Rh$
Exact Mass: 1143.30
Molecular Weight: 1144.00
m/z: 1143.30 (100.0%), 1144.30 (67.1%), 1145.30 (22.1%), 1146.31 (4.8%)

Figure S14. ESI-MS data for **4**. The base peak (m/z = 960 corresponds to fragment A in Figure S13 above. The high mass peak (m/z =1144) corresponds to the fragment above, a hydrated fragment generated (water acquired during the injection).

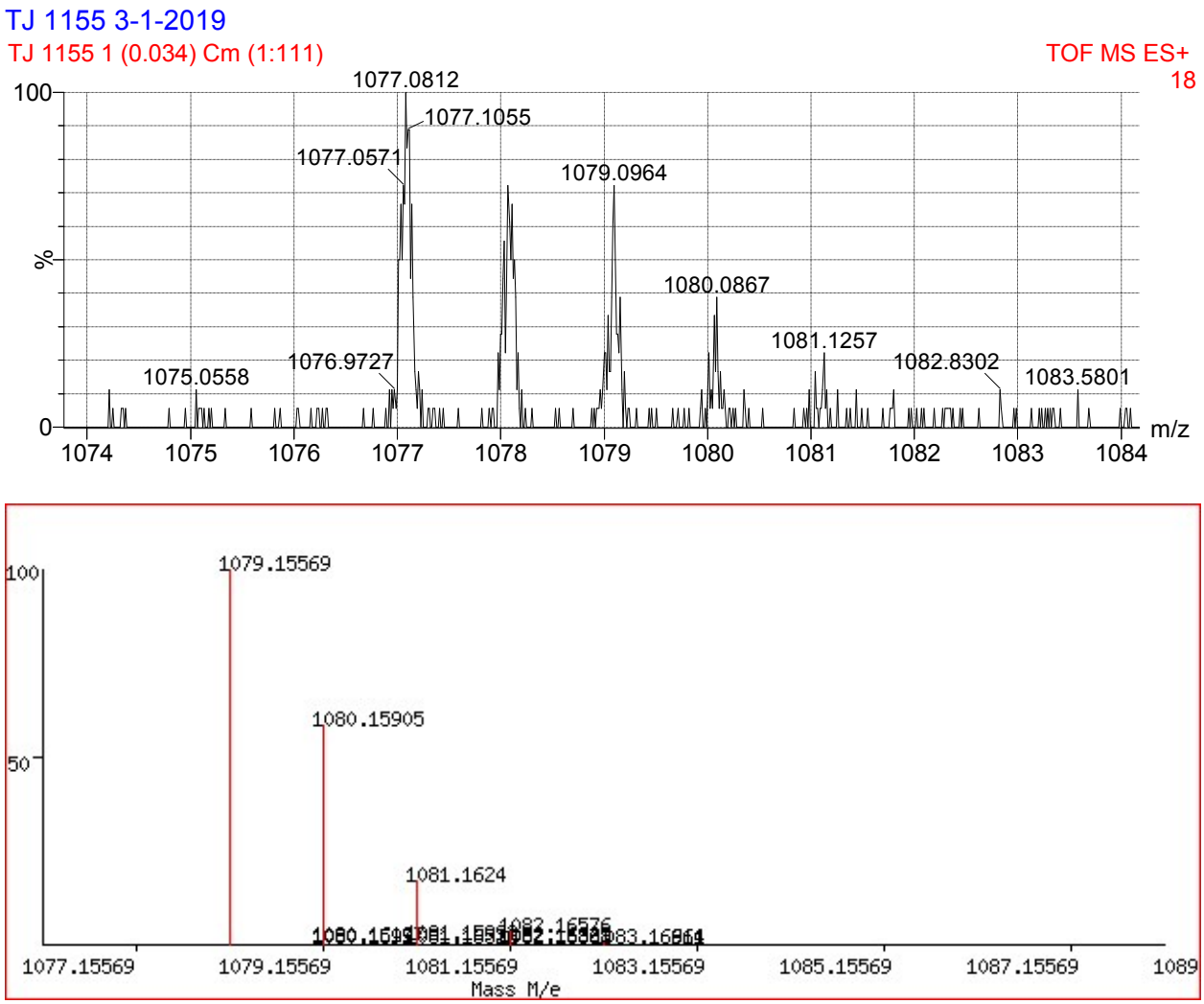


Figure S15. HRMS data for **4**. Top: measured data. Bottom: predicted isotope pattern. Value calculated for $[C_{54}H_{54}Al_2O_6P_4Rh]^+$ (product of alkyl hydrolysis) m/z calc: 1079.1557. Found: 1079.0964. Peaks at 1077 and 1078 correspond to hydrolysis product less two or one hydrogen atoms, respectively.

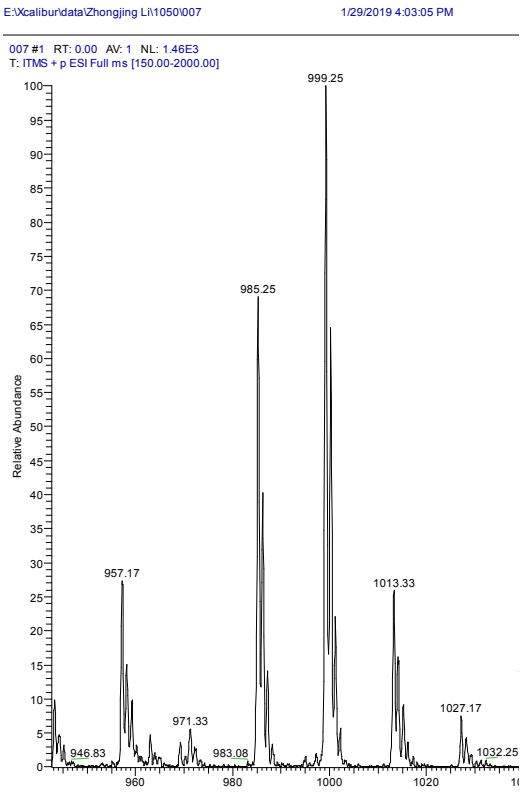
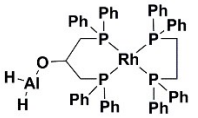
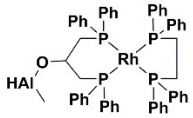


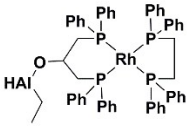
Figure S16. ESI-MS data for **2**. Corresponding fragments are shown below.



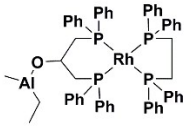
Chemical Formula: $C_{53}H_{51}AlOP_4Rh$
Exact Mass: 957.18
Molecular Weight: 957.77
m/z: 957.18 (100.0%), 958.18 (57.3%), 959.18 (14.5%), 960.19 (2.7%), 959.18 (1.7%)



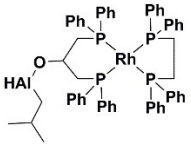
Chemical Formula: $C_{54}H_{53}AlOP_4Rh$
Exact Mass: 971.19
Molecular Weight: 971.80
m/z: 971.19 (100.0%), 972.20 (58.4%), 973.20 (15.1%), 974.20 (2.8%), 973.20 (1.7%)



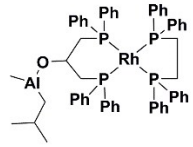
Chemical Formula: $C_{55}H_{55}AlOP_4Rh$
Exact Mass: 985.21
Molecular Weight: 985.83
m/z: 985.21 (100.0%), 986.21 (59.5%), 987.21 (15.7%), 988.22 (3.0%), 987.21 (1.7%)



Chemical Formula: $C_{56}H_{57}AlOP_4Rh$
Exact Mass: 999.22
Molecular Weight: 999.85
m/z: 999.22 (100.0%), 1000.23 (60.6%), 1001.23 (16.4%), 1002.23 (3.1%), 1001.23 (1.7%)



Chemical Formula: $C_{57}H_{59}AlOP_4Rh$
Exact Mass: 1013.24
Molecular Weight: 1013.88
m/z: 1013.24 (100.0%), 1014.24 (61.6%), 1015.25 (17.0%), 1016.25 (3.3%), 1015.25 (1.7%)



Chemical Formula: $C_{58}H_{61}AlOP_4Rh$
Exact Mass: 1027.25
Molecular Weight: 1027.91
m/z: 1027.25 (100.0%), 1028.26 (62.7%), 1029.26 (17.7%), 1030.26 (3.9%), 1029.26 (1.7%)

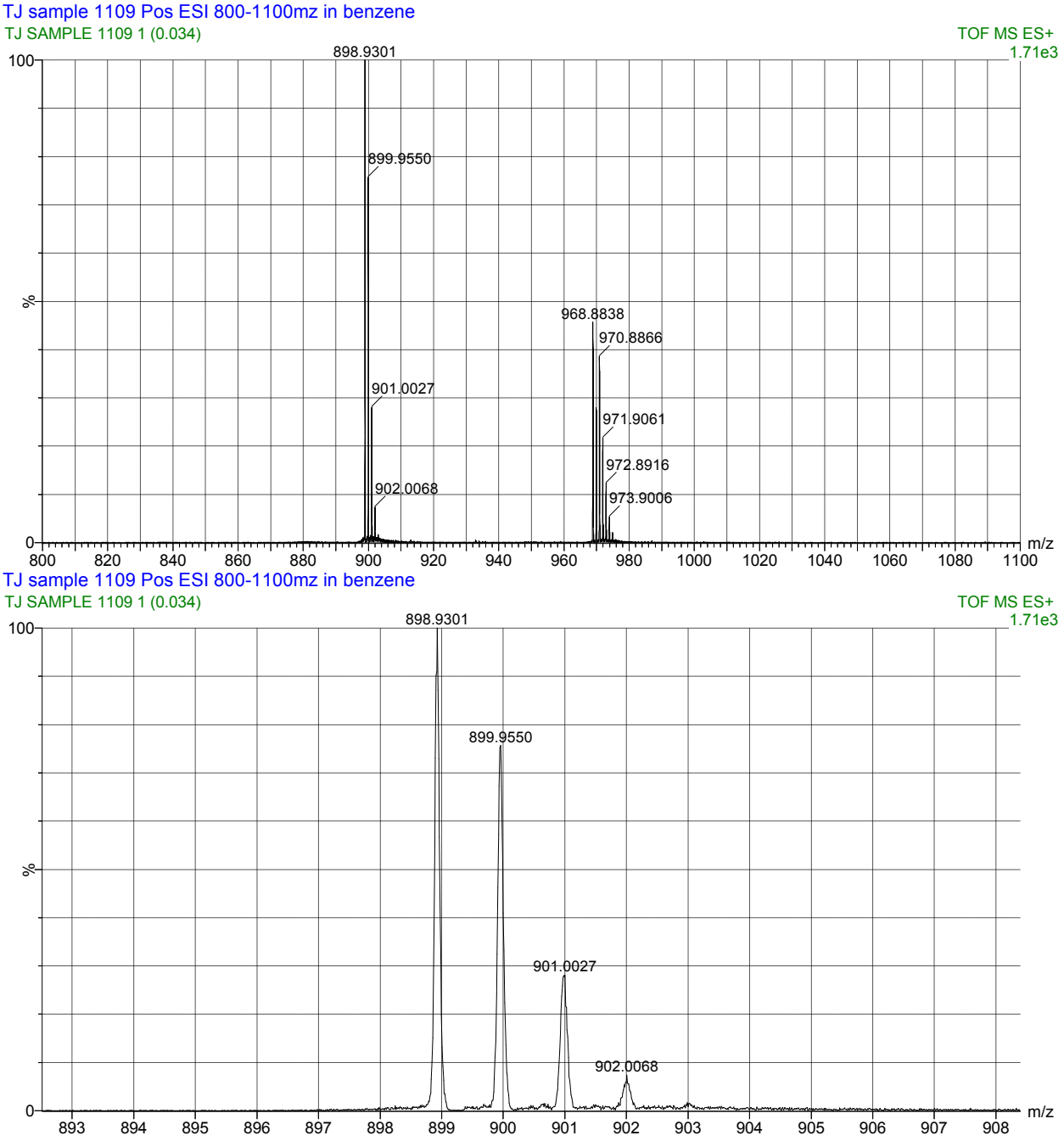


Figure S17a. HRMS data for **2**. Top: Full measured mass spectrum. Bottom: Observed isotope pattern for major impurity $[Rh(DPPE)_2][Cl]$. Value calculated for $[C_{52}H_{48}P_4Rh]^+$ ($M\text{-}Cl^+$) m/z calc: 899.1761. Found: 898.9301.

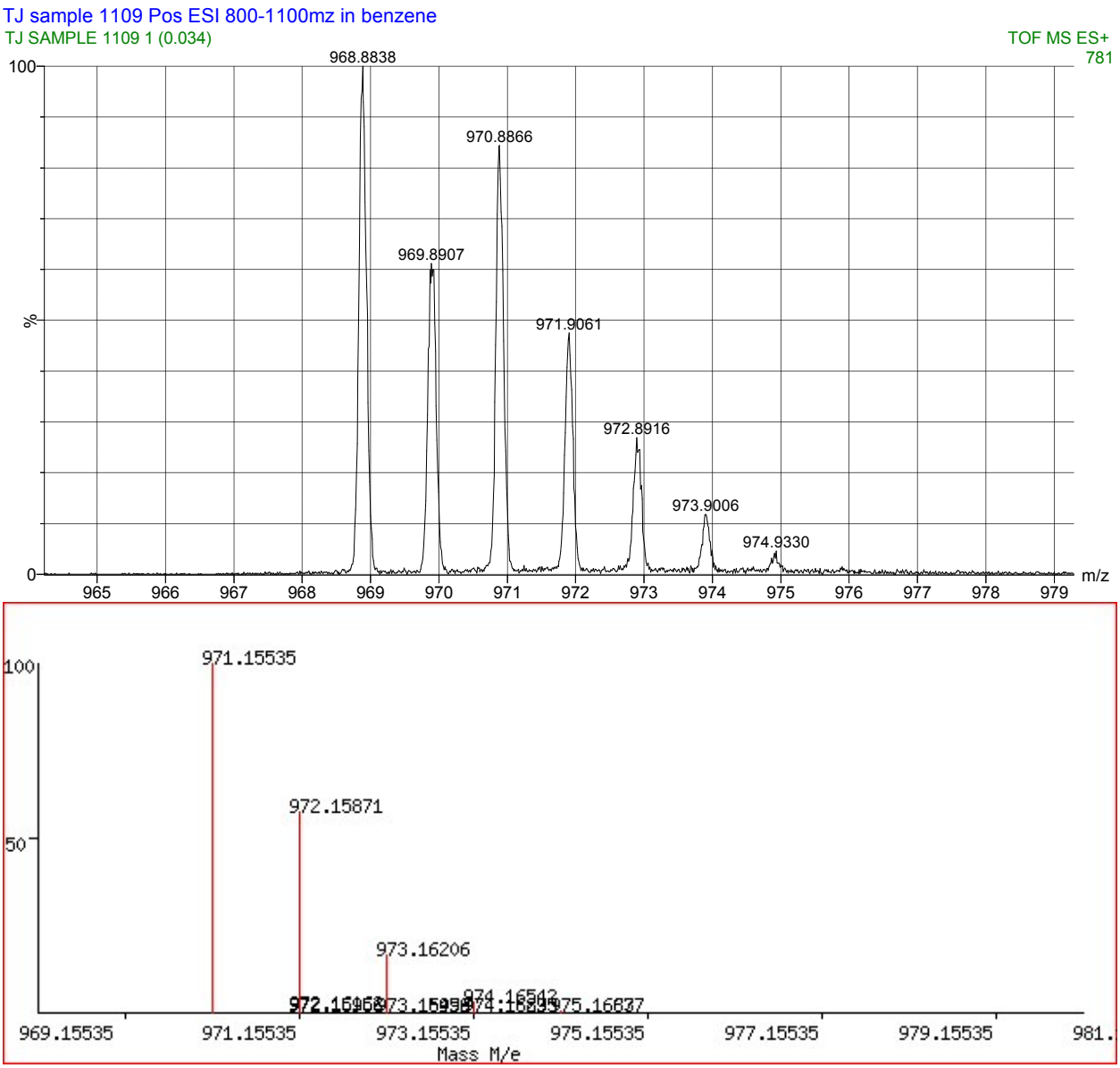


Figure S17b. HRMS data for **2**. Top: measured data. Bottom: predicted isotope pattern. Value calculated for $[C_{53}H_{50}Al_2O_4P_4Rh]^+$ (product of alkyl hydrolysis) m/z calc: 971.1554. Found: 970.8866. Peaks at 969 and 970 correspond to hydrolysis product less two or one hydrogen atoms, respectively.

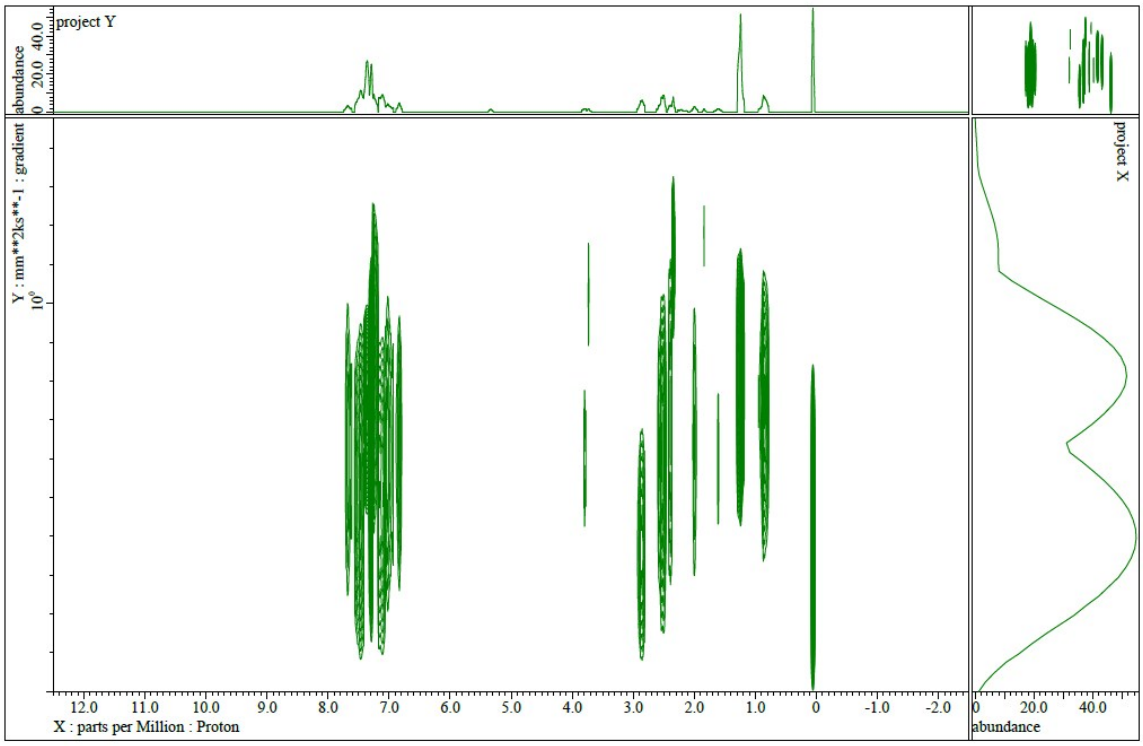


Figure S18: DOSY of [Rh(DPPP-OH)$_2$][Cl] (**3**).

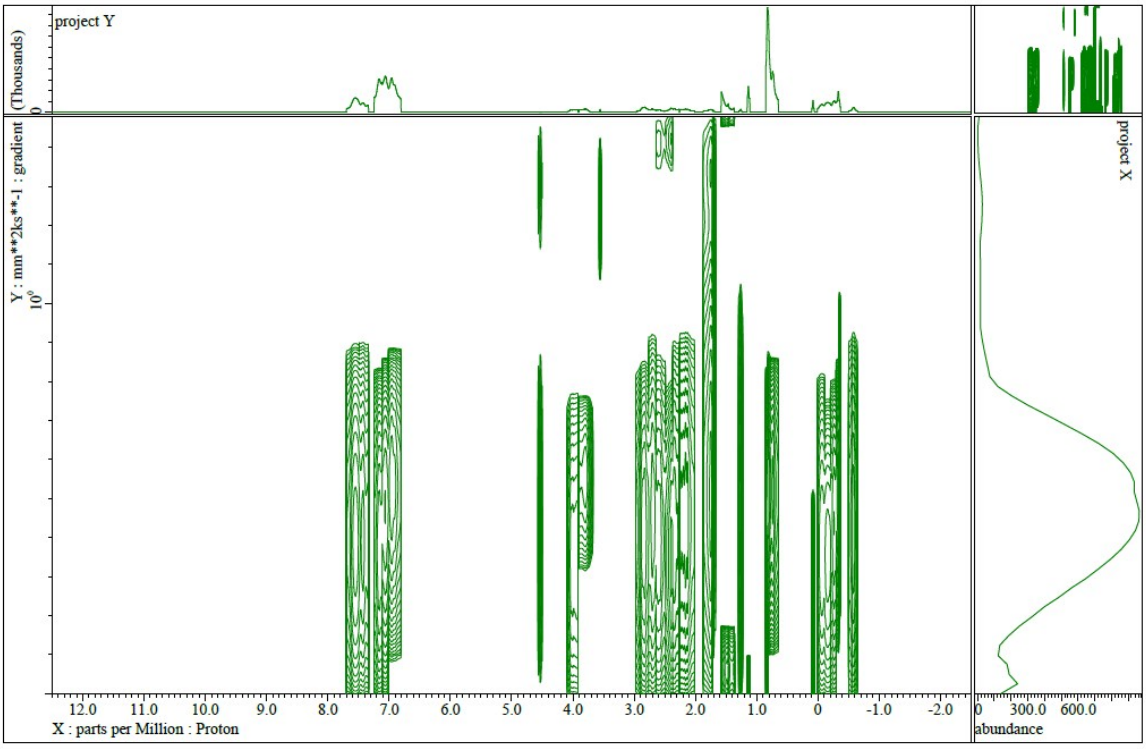


Figure S19: DOSY of Rh(DPPP-OAl^{i}Bu$_2$)(DPPP-OAl^{i}Bu$_2$Cl) (**4**).

X-Ray Crystallography

$Rh(DPPP\text{-}OH)_2(CO)Cl$ (ZL-0048)

The disordered chloroform molecule was modeled over two positions with similarity restraints placed on the C-Cl bond lengths. A single, highly-disordered dichloromethane was modeled over 3 positions using the fragment based approach as Guzei, I. A. (2014). J. Appl. Crystallogr. 47, 806-809. The thermal parameters of all disordered solvent molecules were modeled with similarity restraints.

$[Rh(DPPP\text{-}OH)_2][BArF_{24}]$ (ZL-0051)

Three disordered chloroform molecules were modeled over two positions each with similarity restraints placed on the C-Cl bond lengths and atom thermal parameters. A disordered trifluoromethyl group of the BAr^F_4 anion was modeled over two positions with similarity restraints placed on the C-F bond lengths and atom thermal parameters.

$[Rh(DPPP)_2][Cl]$ (z1dppe)

The structure was modeled without restraint.

Table 1. Crystal data and structure refinement for ZL-0048.

Identification code	zl-0048	
Empirical formula	$C_{55}H_{52}ClO_3P_4Rh \cdot 2(CHCl_3) \cdot 2(CH_2Cl_2)$	
Formula weight	1431.79	
Temperature	100.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 14.88291(13) Å	α = 90°
	b = 20.7830(2) Å	β = 92.8655(7)°
	c = 21.00080(16) Å	γ = 90°
Volume	6487.67(10) $Å^3$	
Z	4	
Density (calculated)	1.466 Mg/m^3	
Absorption coefficient	7.566 mm^{-1}	
F(000)	2912	
Crystal size	0.173 x 0.094 x 0.013 mm^3	
Theta range for data collection	2.993 to 72.273°.	
Index ranges	-18<=h<=17, -23<=k<=25, -24<=l<=17	

Reflections collected	36335
Independent reflections	12419 [R(int) = 0.0370]
Completeness to theta = 67.684°	99.0 %
Absorption correction	Gaussian
Max. and min. transmission	1.000 and 0.490
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12419 / 184 / 790
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0693, wR2 = 0.1859
R indices (all data)	R1 = 0.0805, wR2 = 0.1965
Largest diff. peak and hole	2.358 and -1.352 e/Å^{-3}

Table 2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for ZL-0048. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	47485(2)	66815(2)	39730(2)	182(1)
P(1)	35583(8)	68759(6)	46410(6)	197(3)
P(2)	56217(9)	74257(7)	46197(6)	249(3)
P(3)	41016(8)	72388(6)	30503(6)	226(3)
P(4)	58924(8)	63701(6)	33202(6)	188(2)
O(1)	46100(30)	52786(18)	43456(19)	307(8)
O(2)	38600(40)	86720(20)	53880(30)	524(13)
O(3)	60930(30)	76050(20)	18350(20)	396(10)
C(1)	46550(30)	58050(30)	42050(20)	245(10)
C(2)	36190(30)	65420(20)	54510(20)	215(10)
C(3)	29110(40)	66750(30)	58450(30)	261(11)
C(4)	29440(40)	64660(30)	64720(30)	312(12)
C(5)	36820(40)	61200(30)	67130(30)	300(11)
C(6)	43820(40)	59780(30)	63270(20)	261(11)
C(7)	43440(30)	61850(20)	56930(20)	227(10)
C(8)	24690(30)	65510(30)	43510(20)	236(10)
C(9)	17450(40)	69390(30)	41650(30)	300(11)
C(10)	9510(40)	66610(30)	39090(30)	396(15)
C(11)	8750(40)	60030(30)	38550(30)	380(14)
C(12)	15810(40)	56120(30)	40650(30)	320(12)
C(13)	23760(40)	58860(30)	43130(20)	275(11)
C(14)	33580(40)	77230(20)	48130(20)	254(10)
C(15)	41240(40)	80350(30)	52180(30)	303(12)
C(16)	49990(40)	81340(30)	48800(30)	305(12)
C(17)	60870(30)	70560(30)	53610(30)	304(12)
C(18)	64450(40)	64400(30)	53280(30)	306(12)
C(19)	68100(40)	61410(40)	58760(30)	392(14)
C(20)	68210(40)	64550(40)	64560(30)	472(17)
C(21)	64650(40)	70630(40)	64890(30)	469(17)
C(22)	61070(40)	73730(30)	59450(30)	386(14)
C(23)	66170(40)	78590(30)	43600(30)	382(14)
C(24)	65190(60)	83090(30)	38690(40)	507(18)
C(25)	72550(70)	86460(40)	36680(50)	720(30)

C(26)	80980(60)	85400(50)	39660(50)	740(30)
C(27)	82050(60)	81100(40)	44510(50)	680(30)
C(28)	74740(40)	77620(40)	46560(40)	462(17)
C(29)	33590(40)	79370(30)	31540(20)	280(11)
C(30)	37330(50)	85290(30)	33440(30)	379(13)
C(31)	31850(50)	90450(30)	34880(30)	456(16)
C(32)	22560(50)	89720(40)	34370(30)	471(17)
C(33)	18870(50)	84000(40)	32340(30)	434(16)
C(34)	24290(40)	78800(30)	30930(20)	343(13)
C(35)	34080(40)	67430(30)	24920(30)	277(11)
C(36)	33620(40)	68340(30)	18340(30)	361(13)
C(37)	28120(50)	64550(30)	14430(30)	454(16)
C(38)	22850(50)	59750(30)	16950(30)	424(15)
C(39)	23210(40)	58830(30)	23440(30)	381(13)
C(40)	28760(40)	62570(30)	27370(30)	314(12)
C(41)	48980(40)	76270(30)	25270(30)	284(11)
C(42)	56400(40)	72060(30)	22730(20)	273(11)
C(43)	63210(30)	69830(30)	27940(20)	248(10)
C(44)	56080(30)	57220(20)	27580(20)	217(10)
C(45)	62360(40)	55360(30)	23220(30)	283(11)
C(46)	60200(40)	50660(30)	18690(30)	358(13)
C(47)	51910(40)	47670(30)	18510(30)	373(13)
C(48)	45730(40)	49460(30)	22890(30)	344(13)
C(49)	47730(30)	54200(30)	27350(20)	264(11)
C(50)	69130(30)	60630(20)	37310(20)	218(10)
C(51)	76750(30)	64450(30)	38320(30)	263(11)
C(52)	84170(40)	62040(30)	41850(30)	340(12)
C(53)	84150(40)	55840(30)	44170(30)	341(12)
C(54)	76670(40)	51970(30)	43050(30)	326(12)
C(55)	69100(30)	54400(30)	39660(20)	258(11)
Cl(7)	51782(16)	83018(12)	72170(11)	694(6)
Cl(8)	41205(15)	73532(11)	78894(9)	646(5)
C(58)	43510(50)	76790(40)	71450(40)	540(18)
Cl(5)	107960(90)	86950(70)	46440(50)	1250(40)
Cl(6)	96770(80)	90930(70)	55530(70)	1370(40)
Cl(9)	97660(30)	88660(20)	57894(17)	495(9)
Cl(9B)	101660(90)	76850(50)	53760(40)	1560(40)
Cl(10)	106970(40)	84460(30)	46790(40)	940(20)
Cl(11)	110220(60)	97280(40)	50530(30)	1430(30)
C(59)	107560(110)	89610(70)	53580(70)	920(40)

C(59B)	105220(160)	85000(70)	54280(90)	1020(40)
Cl(1)	24225(11)	83798(8)	63254(8)	471(4)
Cl(2)	53710(30)	93616(18)	17092(16)	1125(11)
Cl(3)	55449(11)	89656(11)	4294(10)	602(5)
Cl(4)	39707(14)	86081(16)	10864(15)	1001(11)
Cl(6B)	37870(160)	102690(110)	48470(100)	1220(60)
Cl(5B)	52100(130)	98510(60)	40230(70)	1080(40)
C(57B)	48600(200)	99200(300)	48080(70)	1310(60)
Cl(6C)	34040(100)	104130(40)	49240(50)	630(30)
Cl(5C)	50450(110)	101620(130)	42460(120)	1800(60)
C(57C)	44800(200)	100500(300)	49530(130)	1270(60)
Cl(12)	63310(40)	104900(50)	24760(30)	1850(50)
Cl(13)	51170(50)	99290(30)	33840(40)	1310(30)
C(57)	61190(120)	103580(150)	32830(30)	1580(70)
C(56)	51270(60)	87410(50)	11430(40)	730(30)

Table 3. Bond lengths [Å] for ZL-0048.

Rh(1)-P(1)	2.3489(12)
Rh(1)-P(2)	2.3978(13)
Rh(1)-P(3)	2.4159(13)
Rh(1)-P(4)	2.3302(12)
Rh(1)-C(1)	1.892(5)
P(1)-C(2)	1.835(5)
P(1)-C(8)	1.832(5)
P(1)-C(14)	1.824(5)
P(2)-C(16)	1.837(6)
P(2)-C(17)	1.839(6)
P(2)-C(23)	1.840(6)
P(3)-C(29)	1.844(5)
P(3)-C(35)	1.839(6)
P(3)-C(41)	1.843(5)
P(4)-C(43)	1.822(5)
P(4)-C(44)	1.827(5)
P(4)-C(50)	1.824(5)
O(1)-C(1)	1.137(7)
O(2)-H(2)	0.8200
O(2)-C(15)	1.430(7)
O(3)-H(3)	0.8200
O(3)-C(42)	1.431(6)
C(2)-C(3)	1.399(7)
C(2)-C(7)	1.385(7)
C(3)-H(3A)	0.9300
C(3)-C(4)	1.387(7)
C(4)-H(4)	0.9300
C(4)-C(5)	1.387(8)
C(5)-H(5)	0.9300
C(5)-C(6)	1.383(8)
C(6)-H(6)	0.9300
C(6)-C(7)	1.396(7)
C(7)-H(7)	0.9300
C(8)-C(9)	1.387(8)
C(8)-C(13)	1.391(8)
C(9)-H(9)	0.9300
C(9)-C(10)	1.398(8)
C(10)-H(10)	0.9300

C(10)-C(11)	1.376(10)
C(11)-H(11)	0.9300
C(11)-C(12)	1.383(9)
C(12)-H(12)	0.9300
C(12)-C(13)	1.391(8)
C(13)-H(13)	0.9300
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(14)-C(15)	1.532(8)
C(15)-H(15)	0.9800
C(15)-C(16)	1.528(7)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.392(9)
C(17)-C(22)	1.392(8)
C(18)-H(18)	0.9300
C(18)-C(19)	1.393(9)
C(19)-H(19)	0.9300
C(19)-C(20)	1.381(9)
C(20)-H(20)	0.9300
C(20)-C(21)	1.373(11)
C(21)-H(21)	0.9300
C(21)-C(22)	1.394(10)
C(22)-H(22)	0.9300
C(23)-C(24)	1.393(10)
C(23)-C(28)	1.406(10)
C(24)-H(24)	0.9300
C(24)-C(25)	1.384(10)
C(25)-H(25)	0.9300
C(25)-C(26)	1.392(15)
C(26)-H(26)	0.9300
C(26)-C(27)	1.358(15)
C(27)-H(27)	0.9300
C(27)-C(28)	1.392(9)
C(28)-H(28)	0.9300
C(29)-C(30)	1.399(9)
C(29)-C(34)	1.388(8)
C(30)-H(30)	0.9300
C(30)-C(31)	1.390(8)
C(31)-H(31)	0.9300

C(31)-C(32)	1.388(11)
C(32)-H(32)	0.9300
C(32)-C(33)	1.370(11)
C(33)-H(33)	0.9300
C(33)-C(34)	1.389(8)
C(34)-H(34)	0.9300
C(35)-C(36)	1.394(8)
C(35)-C(40)	1.396(8)
C(36)-H(36)	0.9300
C(36)-C(37)	1.378(9)
C(37)-H(37)	0.9300
C(37)-C(38)	1.389(10)
C(38)-H(38)	0.9300
C(38)-C(39)	1.375(9)
C(39)-H(39)	0.9300
C(39)-C(40)	1.378(8)
C(40)-H(40)	0.9300
C(41)-H(41A)	0.9700
C(41)-H(41B)	0.9700
C(41)-C(42)	1.526(7)
C(42)-H(42)	0.9800
C(42)-C(43)	1.527(7)
C(43)-H(43A)	0.9700
C(43)-H(43B)	0.9700
C(44)-C(45)	1.394(7)
C(44)-C(49)	1.391(7)
C(45)-H(45)	0.9300
C(45)-C(46)	1.390(8)
C(46)-H(46)	0.9300
C(46)-C(47)	1.381(9)
C(47)-H(47)	0.9300
C(47)-C(48)	1.385(9)
C(48)-H(48)	0.9300
C(48)-C(49)	1.382(8)
C(49)-H(49)	0.9300
C(50)-C(51)	1.393(7)
C(50)-C(55)	1.386(7)
C(51)-H(51)	0.9300
C(51)-C(52)	1.393(8)
C(52)-H(52)	0.9300

C(52)-C(53)	1.378(9)
C(53)-H(53)	0.9300
C(53)-C(54)	1.383(8)
C(54)-H(54)	0.9300
C(54)-C(55)	1.398(7)
C(55)-H(55)	0.9300
Cl(7)-C(58)	1.788(8)
Cl(8)-C(58)	1.752(8)
C(58)-H(58A)	0.9700
C(58)-H(58B)	0.9700
Cl(5)-C(59B)	1.764(14)
Cl(6)-C(59B)	1.788(14)
Cl(9)-C(59)	1.779(12)
Cl(9B)-C(59B)	1.775(15)
Cl(10)-C(59)	1.781(12)
Cl(11)-C(59)	1.770(13)
C(59)-H(59)	0.9800
C(59B)-H(59B)	0.9800
Cl(2)-C(56)	1.779(12)
Cl(3)-C(56)	1.715(8)
Cl(4)-C(56)	1.741(9)
Cl(6B)-C(57B)	1.7602
Cl(5B)-C(57B)	1.7605
C(57B)-H(57A)	0.9700
C(57B)-H(57B)	0.9700
Cl(6C)-C(57C)	1.7598
Cl(5C)-C(57C)	1.7603
C(57C)-H(57C)	0.9700
C(57C)-H(57D)	0.9700
Cl(12)-C(57)	1.7604
Cl(13)-C(57)	1.7596
C(57)-H(57E)	0.9700
C(57)-H(57F)	0.9700
C(56)-H(56)	0.9800

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for ZL-0048. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	176(2)	209(2)	163(2)	8(1)	41(1)	-6(1)
P(1)	187(6)	224(6)	184(6)	16(4)	50(4)	7(5)
P(2)	243(6)	268(6)	244(6)	-57(5)	76(5)	-71(5)
P(3)	238(6)	244(6)	201(6)	47(5)	58(4)	36(5)
P(4)	170(5)	220(6)	176(5)	15(4)	44(4)	-12(4)
O(1)	350(20)	230(20)	350(20)	45(16)	83(16)	-3(16)
O(2)	630(30)	390(30)	580(30)	-140(20)	310(20)	-60(20)
O(3)	410(20)	430(20)	370(20)	211(19)	210(18)	92(19)
C(1)	230(20)	290(30)	220(20)	-10(20)	71(18)	0(20)
C(2)	210(20)	230(20)	200(20)	2(18)	9(18)	-7(19)
C(3)	250(30)	300(30)	230(30)	40(20)	30(20)	20(20)
C(4)	370(30)	350(30)	230(30)	50(20)	100(20)	30(20)
C(5)	400(30)	310(30)	200(20)	50(20)	20(20)	-40(20)
C(6)	260(30)	250(30)	270(30)	20(20)	-20(20)	10(20)
C(7)	230(20)	240(20)	210(20)	10(19)	19(18)	-11(19)
C(8)	210(20)	330(30)	170(20)	30(19)	42(18)	10(20)
C(9)	290(30)	360(30)	250(30)	50(20)	30(20)	40(20)
C(10)	250(30)	560(40)	370(30)	70(30)	-70(20)	110(30)
C(11)	210(30)	550(40)	370(30)	-10(30)	-40(20)	-40(30)
C(12)	290(30)	360(30)	310(30)	-20(20)	40(20)	-70(20)
C(13)	220(20)	350(30)	250(30)	30(20)	41(19)	10(20)
C(14)	290(30)	250(30)	240(20)	-2(19)	110(20)	30(20)
C(15)	390(30)	250(30)	270(30)	-70(20)	120(20)	-30(20)
C(16)	330(30)	270(30)	320(30)	-40(20)	150(20)	-80(20)
C(17)	190(20)	440(30)	280(30)	-80(20)	36(19)	-90(20)
C(18)	230(30)	440(30)	250(30)	-60(20)	20(20)	-30(20)
C(19)	250(30)	580(40)	350(30)	-20(30)	-40(20)	10(30)
C(20)	360(30)	780(50)	270(30)	-40(30)	-40(20)	80(30)
C(21)	370(30)	730(50)	300(30)	-180(30)	-20(20)	-30(30)
C(22)	310(30)	530(40)	330(30)	-140(30)	20(20)	-40(30)
C(23)	400(30)	340(30)	420(30)	-160(30)	190(30)	-160(30)
C(24)	590(40)	440(40)	510(40)	-60(30)	270(30)	-220(30)
C(25)	880(70)	550(50)	780(60)	-90(40)	460(50)	-360(50)
C(26)	560(50)	620(50)	1090(80)	-250(50)	480(50)	-340(40)
C(27)	430(40)	600(50)	1050(70)	-300(50)	330(40)	-320(40)

C(28)	330(30)	460(40)	610(40)	-190(30)	180(30)	-150(30)
C(29)	350(30)	290(30)	200(20)	50(20)	70(20)	90(20)
C(30)	450(30)	310(30)	390(30)	70(30)	110(30)	70(30)
C(31)	700(50)	280(30)	400(30)	60(30)	150(30)	200(30)
C(32)	620(40)	510(40)	290(30)	50(30)	30(30)	330(30)
C(33)	420(40)	600(40)	270(30)	-10(30)	-20(20)	280(30)
C(34)	380(30)	470(40)	180(20)	50(20)	0(20)	130(30)
C(35)	260(30)	310(30)	260(30)	30(20)	30(20)	70(20)
C(36)	490(40)	380(30)	210(30)	50(20)	10(20)	40(30)
C(37)	640(40)	470(40)	240(30)	-10(30)	-60(30)	80(30)
C(38)	470(40)	440(40)	340(30)	-60(30)	-110(30)	10(30)
C(39)	330(30)	430(30)	380(30)	-40(30)	30(20)	-30(30)
C(40)	280(30)	400(30)	270(30)	30(20)	30(20)	20(20)
C(41)	350(30)	260(30)	250(30)	90(20)	80(20)	30(20)
C(42)	290(30)	330(30)	210(20)	100(20)	80(20)	40(20)
C(43)	250(20)	240(20)	260(30)	40(20)	57(19)	-10(20)
C(44)	230(20)	240(20)	180(20)	41(18)	-2(18)	-1(19)
C(45)	300(30)	280(30)	280(30)	-10(20)	80(20)	10(20)
C(46)	410(30)	380(30)	280(30)	-40(20)	80(20)	70(30)
C(47)	480(40)	350(30)	290(30)	-90(20)	-50(20)	10(30)
C(48)	280(30)	380(30)	370(30)	-60(20)	-60(20)	-60(20)
C(49)	230(20)	320(30)	230(20)	0(20)	-6(19)	20(20)
C(50)	200(20)	270(30)	180(20)	-18(19)	53(17)	-7(19)
C(51)	230(20)	290(30)	280(30)	0(20)	60(20)	-40(20)
C(52)	210(30)	410(30)	400(30)	-40(30)	-10(20)	-70(20)
C(53)	200(20)	460(30)	350(30)	-10(30)	-60(20)	40(20)
C(54)	310(30)	340(30)	320(30)	50(20)	-30(20)	30(20)
C(55)	190(20)	340(30)	240(20)	20(20)	-11(18)	-20(20)
Cl(7)	740(14)	764(14)	586(12)	-221(10)	94(10)	-188(11)
Cl(8)	696(12)	792(14)	456(10)	-125(9)	112(8)	-158(11)
C(58)	440(40)	690(50)	490(40)	-40(40)	30(30)	-90(40)
Cl(5)	1360(70)	1780(80)	640(40)	570(50)	210(40)	300(60)
Cl(6)	1040(60)	1550(90)	1540(90)	-660(70)	280(70)	-160(60)
Cl(9)	490(17)	660(20)	339(16)	-95(13)	38(12)	12(15)
Cl(9B)	2300(90)	1360(70)	940(50)	-120(50)	-840(60)	160(70)
Cl(10)	500(20)	1190(40)	1160(40)	-680(40)	270(20)	-80(30)
Cl(11)	1740(70)	1700(70)	880(40)	340(40)	300(40)	250(50)
C(59)	760(60)	1270(80)	750(60)	-160(70)	150(60)	100(70)
C(59B)	960(70)	1290(80)	820(70)	-150(70)	60(70)	130(70)
Cl(1)	441(8)	500(9)	497(9)	-73(7)	270(7)	-13(7)

Cl(2)	1440(30)	1070(20)	890(20)	194(17)	323(19)	380(20)
Cl(3)	354(8)	811(13)	643(11)	340(10)	49(7)	-27(8)
Cl(4)	384(10)	1320(20)	1320(20)	930(20)	233(12)	173(12)
Cl(6B)	1860(140)	830(100)	940(90)	-60(80)	-150(100)	-330(100)
Cl(5B)	1900(100)	410(50)	920(80)	-240(50)	-70(70)	-510(60)
C(57B)	1930(130)	840(100)	1130(110)	-80(100)	-140(110)	-310(110)
Cl(6C)	1250(90)	220(30)	410(40)	-90(30)	-30(50)	-60(40)
Cl(5C)	2220(110)	1300(100)	1870(110)	-60(100)	-60(100)	-400(100)
C(57C)	1860(130)	820(100)	1100(100)	-60(100)	-180(110)	-250(110)
Cl(12)	690(30)	3940(140)	940(40)	-1020(60)	320(30)	-890(60)
Cl(13)	1460(60)	730(40)	1790(70)	-190(40)	460(50)	-400(40)
C(57)	870(110)	2370(150)	1510(130)	-580(130)	250(110)	-540(120)
C(56)	550(50)	940(70)	720(60)	500(50)	230(40)	250(50)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for ZL-0048.

	x	y	z	U(eq)
H(2)	3438	8652	5623	79
H(3)	6528	7411	1706	59
H(3A)	2415	6906	5684	31
H(4)	2471	6558	6732	37
H(5)	3706	5983	7135	36
H(6)	4876	5746	6489	31
H(7)	4809	6082	5432	27
H(9)	1787	7383	4210	36
H(10)	471	6922	3774	48
H(11)	350	5821	3677	46
H(12)	1524	5167	4041	38
H(13)	2850	5622	4455	33
H(14A)	3278	7956	4414	31
H(14B)	2805	7760	5036	31
H(15)	4245	7781	5606	36
H(16A)	5402	8381	5163	37
H(16B)	4862	8398	4508	37
H(18)	6441	6226	4939	37
H(19)	7047	5729	5851	47
H(20)	7068	6257	6821	57
H(21)	6463	7271	6881	56
H(22)	5883	7789	5973	46
H(24)	5953	8382	3674	61
H(25)	7186	8942	3337	87
H(26)	8594	8766	3832	89
H(27)	8771	8048	4648	82
H(28)	7553	7466	4987	55
H(30)	4355	8577	3374	45
H(31)	3438	9436	3618	55
H(32)	1885	9313	3540	57
H(33)	1265	8359	3190	52
H(34)	2169	7494	2958	41

H(36)	3706	7155	1657	43
H(37)	2793	6521	1005	54
H(38)	1915	5720	1429	51
H(39)	1967	5566	2519	46
H(40)	2897	6185	3174	38
H(41A)	4556	7808	2165	34
H(41B)	5182	7982	2760	34
H(42)	5375	6833	2048	33
H(43A)	6513	7352	3049	30
H(43B)	6846	6814	2595	30
H(45)	6801	5727	2335	34
H(46)	6439	4952	1575	43
H(47)	5051	4450	1549	45
H(48)	4014	4744	2283	41
H(49)	4347	5538	3022	32
H(51)	7689	6859	3664	32
H(52)	8919	6464	4265	41
H(53)	8915	5426	4650	41
H(54)	7669	4776	4456	39
H(55)	6402	5183	3898	31
H(58A)	3801	7852	6945	65
H(58B)	4565	7340	6873	65
H(59)	11267	8820	5635	111
H(59B)	11041	8551	5730	123
H(57A)	4859	9501	5004	157
H(57B)	5294	10187	5052	157
H(57C)	4412	9596	5032	152
H(57D)	4835	10235	5307	152
H(57E)	6618	10120	3483	189
H(57F)	6084	10770	3497	189
H(56)	5428	8345	1290	87

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Table 6. Crystal data and structure refinement for ZL-0051.

Identification code	zl-0051	
Empirical formula	$C_{86}H_{64}BF_{24}O_2P_4Rh \cdot (CHCl_3)_3$	
Formula weight	2181.07	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.4257(6) Å	α = 82.035(4)°
	b = 19.1875(10) Å	β = 76.317(4)°
	c = 22.2983(10) Å	γ = 79.953(4)°
Volume	4652.7(4) $Å^3$	
Z	2	
Density (calculated)	1.557 Mg/m^3	
Absorption coefficient	5.357 mm^{-1}	
F(000)	2192	
Crystal size	0.184 x 0.07 x 0.02 mm^3	
Theta range for data collection	2.351 to 72.304°.	
Index ranges	-14<=h<=13, -21<=k<=23, -27<=l<=18	
Reflections collected	40515	
Independent reflections	17273 [R(int) = 0.0586]	
Completeness to theta = 67.684°	96.5 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.449	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17273 / 406 / 1320	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0929, wR2 = 0.2224	
R indices (all data)	R1 = 0.1239, wR2 = 0.2448	
Largest diff. peak and hole	2.746 and -1.504 $e/Å^{-3}$	

Table 7. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for ZL-0051. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	20336(5)	23588(3)	27640(2)	318(2)
P(1)	4119(17)	19780(9)	34828(8)	346(4)
P(2)	6927(17)	28854(9)	21545(8)	344(4)
P(3)	31154(17)	25955(9)	34365(8)	336(4)
P(4)	38141(16)	22910(8)	20035(8)	319(4)
O(1)	-27030(50)	33220(30)	33080(30)	512(14)
O(2)	60120(50)	35390(30)	23810(30)	461(13)
C(1)	5440(70)	15850(40)	42680(40)	402(16)
C(2)	3020(80)	20070(50)	47550(40)	489(19)
C(3)	4250(90)	16930(60)	53440(40)	620(20)
C(4)	7800(90)	9870(60)	54450(40)	650(30)
C(5)	10290(90)	5620(50)	49680(50)	620(30)
C(6)	9070(80)	8650(50)	43750(40)	520(20)
C(7)	-780(60)	12490(40)	32040(30)	354(15)
C(8)	7310(80)	8670(40)	27590(40)	550(20)
C(9)	4010(100)	2830(50)	25560(50)	680(30)
C(10)	-7280(80)	920(40)	27830(40)	520(20)
C(11)	-15360(80)	4720(50)	32270(40)	550(20)
C(12)	-12080(80)	10470(40)	34290(40)	490(20)
C(13)	-10010(70)	26060(40)	36570(30)	390(16)
C(14)	-15270(70)	29120(40)	30970(30)	394(16)
C(15)	-6960(70)	33620(40)	26190(30)	404(17)
C(16)	12490(70)	36630(40)	16680(30)	384(16)
C(17)	10510(70)	38690(40)	10770(30)	389(16)
C(18)	14910(80)	44760(40)	7430(40)	456(19)
C(19)	21370(80)	48700(40)	9930(40)	478(19)
C(20)	23140(90)	46700(40)	15820(40)	510(20)
C(21)	18700(80)	40730(40)	19180(40)	439(18)
C(22)	880(70)	24380(40)	16530(30)	348(15)
C(23)	7690(80)	18190(40)	14120(40)	500(20)
C(24)	3520(90)	14690(50)	10240(50)	620(30)
C(25)	-7410(90)	17010(50)	8690(40)	530(20)
C(26)	-14250(70)	23230(40)	10910(40)	437(18)

C(27)	-10080(70)	26800(40)	14780(30)	416(17)
C(28)	40930(70)	19360(40)	38500(30)	362(15)
C(29)	50180(70)	21150(40)	40870(40)	440(18)
C(30)	57250(70)	16000(40)	43850(40)	440(18)
C(31)	55600(80)	8980(40)	44440(40)	490(20)
C(32)	46650(100)	7120(40)	42140(50)	630(30)
C(33)	39160(80)	12380(40)	39200(40)	490(20)
C(34)	22980(80)	30410(40)	46500(40)	490(20)
C(35)	15440(100)	34740(50)	50800(40)	600(30)
C(36)	6330(90)	39940(40)	49140(40)	560(20)
C(37)	4960(80)	40900(40)	43090(40)	520(20)
C(38)	12580(80)	36630(40)	38690(40)	430(18)
C(39)	21360(70)	31330(40)	40410(30)	389(16)
C(40)	41240(70)	32560(40)	30600(30)	375(16)
C(41)	51820(70)	30210(40)	25350(40)	397(16)
C(42)	47970(70)	29700(40)	19350(30)	366(15)
C(43)	38070(70)	22540(40)	11860(30)	386(16)
C(44)	38920(80)	15970(40)	9620(40)	471(19)
C(45)	38160(90)	15580(40)	3660(40)	520(20)
C(46)	36760(80)	21790(50)	-350(40)	530(20)
C(47)	36140(80)	28300(40)	1780(40)	458(19)
C(48)	36800(70)	28730(40)	7780(30)	419(17)
C(49)	48040(70)	14550(30)	21540(30)	343(15)
C(50)	43030(70)	8690(40)	24810(40)	442(18)
C(51)	50350(80)	2160(40)	25560(40)	510(20)
C(52)	62510(80)	1520(40)	23250(40)	468(19)
C(53)	67580(80)	7180(40)	20020(50)	560(20)
C(54)	60330(80)	13700(40)	19200(50)	540(20)
Cl(7)	-47780(60)	58690(30)	53170(20)	1023(16)
Cl(7B)	-66400(200)	55430(100)	49320(90)	1540(60)
Cl(8)	-71230(70)	62990(50)	50420(30)	1580(30)
Cl(8B)	-69780(190)	70510(100)	47180(80)	1460(60)
Cl(9)	-50210(70)	69140(30)	43190(30)	1300(20)
Cl(9B)	-48700(200)	62480(130)	51050(120)	1690(60)
C(89)	-55400(200)	61540(130)	47150(100)	1310(40)
C(89B)	-59000(300)	63060(180)	46300(180)	1420(50)
Cl(1)	-43830(30)	54382(17)	10770(20)	798(12)
Cl(1B)	-46310(190)	46830(100)	5680(90)	1320(60)
Cl(2)	-22130(40)	48580(20)	14900(30)	1140(20)
Cl(2B)	-40960(170)	52650(80)	15410(80)	1060(40)

Cl(3)	-30790(70)	41340(20)	6727(19)	1090(20)
Cl(3B)	-22530(140)	42960(70)	6980(70)	890(40)
C(87)	-34490(140)	46610(60)	12820(60)	680(30)
C(87B)	-37000(200)	45700(190)	11080(150)	900(50)
Cl(4)	-102100(80)	70210(70)	23930(50)	1770(30)
Cl(4B)	-103530(130)	71720(90)	31380(60)	1770(50)
Cl(5)	-91050(100)	82600(60)	23160(50)	1680(30)
Cl(5B)	-89050(150)	66390(100)	21150(70)	1920(50)
Cl(6)	-88580(60)	74380(60)	31510(30)	1500(30)
Cl(6B)	-99390(100)	81140(80)	20820(50)	1450(40)
C(88)	-90100(300)	74170(160)	24510(130)	1560(40)
C(88B)	-93900(400)	74140(170)	24930(130)	1590(40)
F(1)	-69360(70)	99180(30)	14410(30)	833(19)
F(2)	-79120(110)	97040(40)	8570(70)	1800(60)
F(3)	-60700(130)	97820(40)	5420(50)	2180(80)
F(4)	-79190(90)	67420(70)	10970(60)	1670(50)
F(5)	-74970(120)	72950(40)	2450(50)	1750(60)
F(6)	-62430(60)	64860(30)	5490(40)	890(20)
F(7)	-11790(60)	93990(30)	13700(30)	830(20)
F(8)	-20670(110)	95530(40)	6400(50)	1490(40)
F(9)	-1890(80)	91070(40)	4890(40)	1350(40)
F(10)	2850(60)	66660(30)	1390(30)	830(20)
F(11)	-12440(50)	61110(30)	4470(30)	727(16)
F(12)	-390(60)	60690(30)	10330(30)	794(18)
F(13)	-18590(70)	57680(30)	36010(40)	1010(30)
F(14)	-12870(70)	52540(40)	27850(30)	1010(20)
F(15)	-23100(70)	47450(30)	35840(40)	950(20)
F(16)	-68980(90)	51910(60)	27920(40)	1380(40)
F(17)	-65420(80)	48550(40)	36450(40)	1060(30)
F(18)	-75390(80)	58540(40)	35010(60)	1600(50)
F(19)	-20410(60)	87510(40)	34250(30)	860(20)
F(20)	-26190(90)	79810(40)	41380(50)	1400(40)
F(21)	-33020(80)	90370(60)	42220(40)	1430(40)
F(22)	-80400(130)	81510(100)	39080(90)	1310(50)
F(22B)	-81870(150)	87990(130)	36230(100)	950(50)
F(23)	-80590(140)	92150(100)	36080(80)	910(50)
F(23B)	-74160(150)	96880(100)	36790(90)	1180(60)
F(24)	-75700(200)	87790(150)	44730(70)	1030(50)
F(24B)	-76200(300)	89390(180)	44390(80)	1030(60)
C(0AA)	-72920(190)	89820(150)	38580(110)	970(50)

C(55)	-54040(70)	77800(40)	17080(30)	385(16)
C(56)	-57760(70)	85060(40)	15650(40)	429(17)
C(57)	-64970(80)	87510(40)	11380(40)	500(20)
C(58)	-68920(80)	82770(50)	8380(40)	530(20)
C(59)	-65510(80)	75630(50)	9790(40)	500(20)
C(60)	-58090(70)	73170(40)	14010(40)	455(18)
C(61)	-68330(110)	95320(50)	9820(50)	700(30)
C(62)	-69740(90)	70390(60)	6680(60)	690(30)
C(63)	-31010(70)	76230(40)	16660(30)	389(16)
C(64)	-26930(80)	82840(40)	14940(40)	455(18)
C(65)	-16340(90)	83760(50)	10410(40)	520(20)
C(66)	-9270(80)	78100(50)	7590(40)	510(20)
C(67)	-13180(70)	71500(40)	9210(40)	437(18)
C(68)	-23680(70)	70540(40)	13650(30)	386(16)
C(69)	-12570(110)	90990(50)	8750(60)	740(30)
C(70)	-5730(80)	65050(50)	6350(40)	530(20)
C(71)	-44190(70)	67250(40)	25030(30)	404(17)
C(72)	-33720(80)	63600(40)	27010(40)	449(18)
C(73)	-33770(90)	57100(40)	30640(40)	481(19)
C(74)	-44230(100)	53910(40)	32440(40)	560(20)
C(75)	-54760(90)	57450(40)	30600(40)	510(20)
C(76)	-54450(80)	63960(40)	26970(40)	458(18)
C(77)	-22240(100)	53690(40)	32580(50)	630(30)
C(78)	-66130(110)	54370(50)	32490(50)	660(30)
C(79)	-46640(70)	80180(30)	27260(30)	363(16)
C(80)	-37410(70)	81350(30)	29920(30)	381(16)
C(81)	-39890(70)	84630(40)	35320(30)	401(17)
C(82)	-51610(80)	86890(40)	38370(40)	473(19)
C(83)	-60840(80)	85810(40)	35710(40)	540(20)
C(84)	-58510(70)	82560(40)	30320(40)	414(17)
C(85)	-29660(80)	85540(40)	38140(40)	500(20)
C(86)	-74000(150)	87000(160)	39060(100)	960(40)
B(1)	-44210(80)	75400(40)	21410(40)	382(18)

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Table 8. Bond lengths [Å] for ZL-0051.

Rh(1)-P(1)	2.2976(19)	C(10)-C(11)	1.378(12)
Rh(1)-P(2)	2.2977(19)	C(11)-H(11)	0.9500
Rh(1)-P(3)	2.2899(19)	C(11)-C(12)	1.386(12)
Rh(1)-P(4)	2.3170(18)	C(12)-H(12)	0.9500
P(1)-C(1)	1.837(8)	C(13)-H(13A)	0.9900
P(1)-C(7)	1.827(7)	C(13)-H(13B)	0.9900
P(1)-C(13)	1.834(7)	C(13)-C(14)	1.514(10)
P(2)-C(15)	1.844(7)	C(14)-H(14)	1.0000
P(2)-C(16)	1.833(7)	C(14)-C(15)	1.528(11)
P(2)-C(22)	1.817(7)	C(15)-H(15A)	0.9900
P(3)-C(28)	1.837(7)	C(15)-H(15B)	0.9900
P(3)-C(39)	1.845(7)	C(16)-C(17)	1.383(10)
P(3)-C(40)	1.843(7)	C(16)-C(21)	1.392(11)
P(4)-C(42)	1.833(7)	C(17)-H(17)	0.9500
P(4)-C(43)	1.837(8)	C(17)-C(18)	1.397(11)
P(4)-C(49)	1.834(7)	C(18)-H(18)	0.9500
O(1)-H(1)	0.8400	C(18)-C(19)	1.390(12)
O(1)-C(14)	1.442(9)	C(19)-H(19)	0.9500
O(2)-H(2)	0.8400	C(19)-C(20)	1.369(11)
O(2)-C(41)	1.443(9)	C(20)-H(20)	0.9500
C(1)-C(2)	1.391(11)	C(20)-C(21)	1.385(11)
C(1)-C(6)	1.376(11)	C(21)-H(21)	0.9500
C(2)-H(2A)	0.9500	C(22)-C(23)	1.401(10)
C(2)-C(3)	1.396(12)	C(22)-C(27)	1.384(10)
C(3)-H(3)	0.9500	C(23)-H(23)	0.9500
C(3)-C(4)	1.350(15)	C(23)-C(24)	1.377(12)
C(4)-H(4)	0.9500	C(24)-H(24)	0.9500
C(4)-C(5)	1.376(15)	C(24)-C(25)	1.358(13)
C(5)-H(5)	0.9500	C(25)-H(25)	0.9500
C(5)-C(6)	1.396(12)	C(25)-C(26)	1.391(12)
C(6)-H(6)	0.9500	C(26)-H(26)	0.9500
C(7)-C(8)	1.381(10)	C(26)-C(27)	1.383(11)
C(7)-C(12)	1.372(11)	C(27)-H(27)	0.9500
C(8)-H(8)	0.9500	C(28)-C(29)	1.398(11)
C(8)-C(9)	1.404(12)	C(28)-C(33)	1.371(10)
C(9)-H(9)	0.9500	C(29)-H(29)	0.9500
C(9)-C(10)	1.364(13)	C(29)-C(30)	1.366(11)
C(10)-H(10)	0.9500	C(30)-H(30)	0.9500

C(30)-C(31)	1.377(12)	C(51)-C(52)	1.352(12)
C(31)-H(31)	0.9500	C(52)-H(52)	0.9500
C(31)-C(32)	1.366(13)	C(52)-C(53)	1.356(12)
C(32)-H(32)	0.9500	C(53)-H(53)	0.9500
C(32)-C(33)	1.400(11)	C(53)-C(54)	1.389(11)
C(33)-H(33)	0.9500	C(54)-H(54)	0.9500
C(34)-H(34)	0.9500	Cl(7)-C(89)	1.74(2)
C(34)-C(35)	1.388(11)	Cl(7B)-C(89B)	1.79(3)
C(34)-C(39)	1.397(11)	Cl(8)-C(89)	1.78(3)
C(35)-H(35)	0.9500	Cl(8B)-C(89B)	1.72(3)
C(35)-C(36)	1.390(12)	Cl(9)-C(89)	1.72(2)
C(36)-H(36)	0.9500	Cl(9B)-C(89B)	1.74(3)
C(36)-C(37)	1.377(12)	C(89)-H(89)	1.0000
C(37)-H(37)	0.9500	C(89B)-H(89B)	1.0000
C(37)-C(38)	1.401(11)	Cl(1)-C(87)	1.749(13)
C(38)-H(38)	0.9500	Cl(1B)-C(87B)	1.75(2)
C(38)-C(39)	1.381(10)	Cl(2)-C(87)	1.702(16)
C(40)-H(40A)	0.9900	Cl(2B)-C(87B)	1.69(2)
C(40)-H(40B)	0.9900	Cl(3)-C(87)	1.734(13)
C(40)-C(41)	1.524(10)	Cl(3B)-C(87B)	1.72(2)
C(41)-H(41)	1.0000	C(87)-H(87)	1.0000
C(41)-C(42)	1.523(10)	C(87B)-H(87B)	1.0000
C(42)-H(42A)	0.9900	Cl(4)-C(88)	1.71(3)
C(42)-H(42B)	0.9900	Cl(4B)-C(88B)	1.65(3)
C(43)-C(44)	1.398(11)	Cl(5)-Cl(6)	2.306(15)
C(43)-C(48)	1.400(10)	Cl(5)-C(88)	1.59(3)
C(44)-H(44)	0.9500	Cl(5B)-C(88B)	1.75(3)
C(44)-C(45)	1.364(11)	Cl(6)-C(88)	1.62(3)
C(45)-H(45)	0.9500	Cl(6B)-C(88B)	1.63(3)
C(45)-C(46)	1.398(11)	C(88)-H(88)	1.0000
C(46)-H(46)	0.9500	C(88B)-H(88B)	1.0000
C(46)-C(47)	1.382(12)	F(1)-C(61)	1.315(12)
C(47)-H(47)	0.9500	F(2)-C(61)	1.304(14)
C(47)-C(48)	1.372(11)	F(3)-C(61)	1.252(14)
C(48)-H(48)	0.9500	F(4)-C(62)	1.408(15)
C(49)-C(50)	1.387(10)	F(5)-C(62)	1.234(13)
C(49)-C(54)	1.366(11)	F(6)-C(62)	1.247(11)
C(50)-H(50)	0.9500	F(7)-C(69)	1.342(13)
C(50)-C(51)	1.392(10)	F(8)-C(69)	1.308(15)
C(51)-H(51)	0.9500	F(9)-C(69)	1.318(12)

F(10)-C(70)	1.333(11)	C(67)-C(68)	1.385(11)
F(11)-C(70)	1.332(10)	C(67)-C(70)	1.503(11)
F(12)-C(70)	1.316(11)	C(68)-H(68)	0.9500
F(13)-C(77)	1.330(12)	C(71)-C(72)	1.410(11)
F(14)-C(77)	1.324(12)	C(71)-C(76)	1.379(12)
F(15)-C(77)	1.318(10)	C(71)-B(1)	1.657(10)
F(16)-C(78)	1.307(12)	C(72)-H(72)	0.9500
F(17)-C(78)	1.328(12)	C(72)-C(73)	1.389(11)
F(18)-C(78)	1.275(13)	C(73)-C(74)	1.386(13)
F(19)-C(85)	1.275(10)	C(73)-C(77)	1.498(13)
F(20)-C(85)	1.285(11)	C(74)-H(74)	0.9500
F(21)-C(85)	1.333(11)	C(74)-C(75)	1.396(13)
F(22)-C(86)	1.38(3)	C(75)-C(76)	1.393(11)
F(22B)-C(0AA)	1.37(3)	C(75)-C(78)	1.468(14)
F(23)-C(86)	1.33(3)	C(76)-H(76)	0.9500
F(23B)-C(0AA)	1.35(3)	C(79)-C(80)	1.390(11)
F(24)-C(86)	1.259(19)	C(79)-C(84)	1.395(11)
F(24B)-C(0AA)	1.26(2)	C(79)-B(1)	1.641(11)
C(0AA)-C(83)	1.502(18)	C(80)-H(80)	0.9500
C(55)-C(56)	1.400(10)	C(80)-C(81)	1.383(10)
C(55)-C(60)	1.390(11)	C(81)-C(82)	1.375(12)
C(55)-B(1)	1.618(11)	C(81)-C(85)	1.496(12)
C(56)-H(56)	0.9500	C(82)-H(82)	0.9500
C(56)-C(57)	1.385(11)	C(82)-C(83)	1.384(13)
C(57)-C(58)	1.390(12)	C(83)-C(84)	1.379(12)
C(57)-C(61)	1.495(11)	C(83)-C(86)	1.506(17)
C(58)-H(58)	0.9500	C(84)-H(84)	0.9500
C(58)-C(59)	1.370(12)		
C(59)-C(60)	1.393(11)		
C(59)-C(62)	1.500(13)		
C(60)-H(60)	0.9500		
C(63)-C(64)	1.400(11)		
C(63)-C(68)	1.400(10)		
C(63)-B(1)	1.644(12)		
C(64)-H(64)	0.9500		
C(64)-C(65)	1.401(12)		
C(65)-C(66)	1.367(12)		
C(65)-C(69)	1.497(12)		
C(66)-H(66)	0.9500		
C(66)-C(67)	1.388(12)		

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for ZL-0051. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	414(3)	247(2)	293(3)	-22(2)	-96(2)	-27(2)
P(1)	419(9)	321(8)	308(9)	-51(7)	-100(7)	-42(7)
P(2)	429(10)	280(8)	317(9)	-43(7)	-103(7)	5(7)
P(3)	453(10)	268(8)	311(9)	-18(6)	-126(7)	-66(7)
P(4)	414(9)	237(7)	299(9)	4(6)	-92(7)	-36(6)
O(1)	520(30)	490(30)	550(40)	-180(30)	-150(30)	30(30)
O(2)	520(30)	410(30)	490(30)	10(20)	-150(30)	-170(20)
C(1)	390(40)	450(40)	380(40)	30(30)	-130(30)	-120(30)
C(2)	560(50)	550(50)	390(50)	-70(40)	-120(40)	-110(40)
C(3)	690(60)	810(70)	370(50)	20(40)	-140(40)	-170(50)
C(4)	700(60)	940(80)	370(50)	240(50)	-200(40)	-370(60)
C(5)	710(60)	590(60)	660(60)	180(50)	-330(50)	-280(50)
C(6)	670(50)	500(50)	400(50)	0(40)	-170(40)	-120(40)
C(7)	400(40)	320(30)	330(40)	-10(30)	-70(30)	-30(30)
C(8)	570(50)	420(40)	620(60)	-210(40)	70(40)	-160(40)
C(9)	850(70)	480(50)	670(70)	-340(50)	110(50)	-200(50)
C(10)	690(60)	420(40)	500(50)	-130(40)	-90(40)	-170(40)
C(11)	550(50)	570(50)	570(60)	-180(40)	-60(40)	-190(40)
C(12)	510(50)	520(50)	460(50)	-250(40)	-60(40)	-60(40)
C(13)	470(40)	430(40)	280(40)	-100(30)	-90(30)	-20(30)
C(14)	450(40)	370(40)	350(40)	-80(30)	-100(30)	20(30)
C(15)	520(40)	310(30)	390(40)	-70(30)	-170(30)	40(30)
C(16)	480(40)	300(30)	360(40)	-20(30)	-130(30)	10(30)
C(17)	530(40)	310(30)	340(40)	-50(30)	-120(30)	-20(30)
C(18)	660(50)	360(40)	330(40)	20(30)	-180(40)	0(30)
C(19)	700(50)	310(40)	410(50)	0(30)	-120(40)	-50(30)
C(20)	720(60)	320(40)	520(50)	-10(30)	-230(40)	-80(40)
C(21)	620(50)	280(30)	420(40)	-40(30)	-170(40)	-10(30)
C(22)	450(40)	290(30)	310(40)	-30(30)	-100(30)	-50(30)
C(23)	540(50)	360(40)	650(60)	-190(40)	-210(40)	40(30)
C(24)	600(50)	480(50)	820(70)	-320(50)	-250(50)	100(40)
C(25)	690(60)	510(50)	460(50)	-120(40)	-130(40)	-220(40)
C(26)	370(40)	510(40)	430(50)	-10(30)	-110(30)	-50(30)
C(27)	460(40)	460(40)	340(40)	-50(30)	-150(30)	-10(30)
C(28)	470(40)	320(30)	290(40)	-60(30)	-70(30)	-10(30)

C(29)	500(40)	410(40)	420(40)	-10(30)	-130(30)	-70(30)
C(30)	420(40)	580(50)	320(40)	60(30)	-100(30)	-110(30)
C(31)	620(50)	460(40)	350(40)	30(30)	-150(40)	50(40)
C(32)	980(80)	270(40)	670(60)	50(40)	-310(60)	-30(40)
C(33)	640(50)	350(40)	510(50)	80(30)	-240(40)	-80(40)
C(34)	710(60)	350(40)	420(50)	-120(30)	-190(40)	70(40)
C(35)	900(70)	570(50)	320(50)	-160(40)	-200(40)	90(50)
C(36)	810(60)	360(40)	450(50)	-180(30)	-110(40)	100(40)
C(37)	670(50)	400(40)	490(50)	-110(30)	-200(40)	60(40)
C(38)	630(50)	330(40)	350(40)	-50(30)	-170(40)	-40(30)
C(39)	500(40)	320(30)	340(40)	-80(30)	-110(30)	-20(30)
C(40)	510(40)	310(30)	320(40)	0(30)	-110(30)	-70(30)
C(41)	500(40)	310(30)	390(40)	20(30)	-140(30)	-60(30)
C(42)	430(40)	280(30)	390(40)	10(30)	-100(30)	-70(30)
C(43)	420(40)	370(40)	360(40)	10(30)	-100(30)	-30(30)
C(44)	770(60)	340(40)	310(40)	-30(30)	-130(40)	-80(40)
C(45)	750(60)	390(40)	440(50)	-140(30)	-160(40)	-50(40)
C(46)	660(50)	610(50)	270(40)	0(30)	-120(40)	30(40)
C(47)	640(50)	320(40)	380(40)	-10(30)	-130(40)	40(30)
C(48)	520(40)	340(40)	350(40)	-10(30)	-60(30)	-10(30)
C(49)	460(40)	280(30)	280(40)	-10(30)	-90(30)	-20(30)
C(50)	480(40)	330(40)	450(50)	50(30)	-40(30)	-40(30)
C(51)	650(50)	340(40)	440(50)	100(30)	-80(40)	0(40)
C(52)	600(50)	280(40)	500(50)	-40(30)	-180(40)	60(30)
C(53)	450(50)	360(40)	820(70)	-90(40)	-60(40)	20(30)
C(54)	510(50)	340(40)	710(60)	10(40)	-80(40)	-70(30)
Cl(7)	1520(40)	780(30)	870(30)	200(20)	-440(30)	-430(30)
Cl(7B)	1910(110)	1440(100)	1170(90)	-370(80)	-210(90)	20(100)
Cl(8)	1420(50)	1880(70)	1120(50)	-190(40)	100(40)	190(50)
Cl(8B)	1890(120)	1280(100)	1020(100)	-310(80)	90(90)	-110(100)
Cl(9)	2230(60)	680(30)	960(40)	200(20)	-290(40)	-450(30)
Cl(9B)	2190(100)	1380(100)	1450(100)	-80(90)	-350(90)	-270(100)
C(89)	1790(80)	1210(80)	950(70)	-220(70)	-310(70)	-200(70)
C(89B)	1860(90)	1290(80)	1050(80)	-230(80)	-180(80)	-170(80)
Cl(1)	790(20)	464(16)	1050(30)	50(17)	-230(20)	77(15)
Cl(1B)	1790(120)	1010(90)	1120(100)	-350(80)	-110(100)	-150(90)
Cl(2)	1070(30)	670(20)	1880(50)	530(30)	-870(30)	-420(20)
Cl(2B)	1490(90)	670(70)	930(80)	-230(60)	-40(80)	-50(70)
Cl(3)	2120(60)	479(19)	490(20)	-113(15)	-50(30)	0(30)
Cl(3B)	1150(90)	410(50)	830(70)	220(50)	20(70)	100(60)

C(87)	1040(70)	330(40)	700(60)	-100(40)	-270(50)	-100(50)
C(87B)	1280(80)	500(70)	830(80)	-80(70)	-110(70)	-40(70)
Cl(4)	1080(50)	2750(90)	1790(70)	-1060(60)	-50(50)	-870(60)
Cl(4B)	1450(80)	2290(90)	1380(80)	-420(80)	240(70)	-310(80)
Cl(5)	1270(60)	1980(70)	1640(60)	-60(60)	0(50)	-370(60)
Cl(5B)	1810(90)	2460(110)	1520(90)	-790(80)	-190(80)	-170(90)
Cl(6)	950(40)	2720(70)	1000(40)	-1030(40)	-360(30)	180(50)
Cl(6B)	860(60)	2090(90)	1160(70)	-270(70)	-110(50)	400(60)
C(88)	1100(60)	2310(70)	1320(60)	-640(60)	-160(60)	-150(60)
C(88B)	1140(60)	2320(70)	1340(60)	-620(60)	-140(60)	-140(60)
F(1)	1240(50)	450(30)	770(40)	-80(30)	-290(40)	70(30)
F(2)	2290(120)	640(50)	3080(150)	-380(70)	-2110(130)	400(60)
F(3)	3100(150)	440(40)	1600(90)	360(50)	1440(100)	460(60)
F(4)	1360(80)	2180(120)	1810(110)	-1060(90)	130(70)	-1120(80)
F(5)	3170(150)	690(50)	2160(110)	-310(60)	-2260(120)	50(70)
F(6)	970(50)	690(40)	1280(60)	-560(40)	-640(40)	120(30)
F(7)	1030(50)	480(30)	950(50)	-280(30)	70(40)	-250(30)
F(8)	2180(110)	710(50)	1880(100)	670(60)	-1120(90)	-740(60)
F(9)	1510(70)	930(50)	1360(70)	-600(50)	850(60)	-750(50)
F(10)	930(40)	700(40)	740(40)	-350(30)	260(30)	-160(30)
F(11)	700(30)	630(30)	940(40)	-450(30)	-200(30)	-20(30)
F(12)	810(40)	740(40)	800(40)	-280(30)	-300(30)	320(30)
F(13)	1260(60)	600(40)	1400(70)	-350(40)	-890(50)	200(40)
F(14)	940(50)	1130(60)	810(50)	-80(40)	-270(40)	370(40)
F(15)	1240(60)	420(30)	1260(60)	240(30)	-660(50)	-70(30)
F(16)	1690(80)	2010(100)	830(60)	260(60)	-500(60)	-1350(80)
F(17)	1260(60)	870(50)	1100(60)	330(40)	-300(50)	-570(50)
F(18)	940(60)	740(50)	2850(140)	-470(70)	460(70)	-350(40)
F(19)	800(40)	1280(60)	610(40)	160(40)	-250(30)	-530(40)
F(20)	1820(90)	1120(60)	1730(90)	810(60)	-1420(80)	-790(60)
F(21)	1010(60)	2210(110)	1400(80)	-1310(80)	-280(50)	-220(60)
F(22)	840(80)	1390(110)	1430(100)	-340(90)	360(70)	-150(80)
F(22B)	470(60)	1480(120)	760(80)	-210(100)	0(60)	150(90)
F(23)	540(70)	1280(110)	800(70)	-180(90)	-100(50)	160(80)
F(23B)	720(80)	1190(110)	1210(100)	30(90)	150(80)	380(80)
F(24)	730(70)	1600(120)	520(70)	-80(80)	30(60)	210(80)
F(24B)	810(90)	1540(120)	560(80)	-370(80)	40(80)	280(90)
C(0AA)	600(60)	1340(100)	810(70)	-200(80)	-10(60)	170(70)
C(55)	510(40)	290(30)	340(40)	-70(30)	-100(30)	0(30)
C(56)	510(40)	350(40)	440(50)	-40(30)	-120(30)	-50(30)

C(57)	630(50)	340(40)	560(50)	-50(30)	-240(40)	-10(30)
C(58)	600(50)	520(50)	530(50)	-40(40)	-310(40)	20(40)
C(59)	510(50)	490(50)	600(50)	-90(40)	-250(40)	-70(40)
C(60)	490(40)	350(40)	550(50)	-50(30)	-130(40)	-70(30)
C(61)	1020(80)	380(50)	700(70)	-30(40)	-370(60)	160(50)
C(62)	580(60)	600(60)	1000(90)	-130(60)	-360(60)	-70(50)
C(63)	490(40)	340(40)	350(40)	-50(30)	-170(30)	20(30)
C(64)	640(50)	320(40)	400(40)	-130(30)	-90(40)	-30(30)
C(65)	710(60)	470(50)	420(50)	-80(40)	-110(40)	-140(40)
C(66)	550(50)	530(50)	470(50)	-130(40)	-30(40)	-120(40)
C(67)	510(40)	460(40)	390(40)	-150(30)	-160(30)	-30(30)
C(68)	460(40)	330(30)	400(40)	-90(30)	-180(30)	10(30)
C(69)	900(80)	500(60)	760(80)	-180(50)	120(60)	-310(50)
C(70)	450(40)	600(50)	540(50)	-190(40)	-110(40)	10(40)
C(71)	590(50)	260(30)	350(40)	-90(30)	-100(30)	10(30)
C(72)	630(50)	290(40)	430(50)	-100(30)	-120(40)	-30(30)
C(73)	730(60)	340(40)	390(40)	-70(30)	-170(40)	-40(40)
C(74)	980(70)	280(40)	420(50)	-80(30)	-140(50)	-110(40)
C(75)	660(50)	380(40)	500(50)	-70(30)	-70(40)	-140(40)
C(76)	570(50)	400(40)	420(50)	-130(30)	-120(40)	-40(30)
C(77)	940(70)	320(40)	610(60)	-10(40)	-220(50)	20(40)
C(78)	960(80)	530(50)	530(60)	-90(40)	-110(50)	-250(50)
C(79)	480(40)	230(30)	370(40)	20(30)	-110(30)	-40(30)
C(80)	490(40)	250(30)	390(40)	-30(30)	-90(30)	-30(30)
C(81)	590(50)	240(30)	350(40)	0(30)	-110(30)	-50(30)
C(82)	730(60)	350(40)	310(40)	-10(30)	-120(40)	0(40)
C(83)	580(50)	440(40)	440(50)	30(40)	40(40)	70(40)
C(84)	490(40)	350(40)	410(40)	0(30)	-130(30)	-40(30)
C(85)	600(50)	450(40)	500(50)	-90(40)	-150(40)	-150(40)
C(86)	580(60)	1350(100)	800(70)	-200(80)	-40(60)	140(70)
B(1)	520(50)	230(30)	390(50)	-60(30)	-120(40)	20(30)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ZL-0051.

	x	y	z	U(eq)
H(1)	-2615	3679	3463	77
H(2)	6087	3680	2709	69
H(2A)	55	2505	4686	59
H(3)	256	1980	5678	74
H(4)	860	780	5849	79
H(5)	1283	65	5041	75
H(6)	1074	572	4045	62
H(8)	1515	1000	2589	66
H(9)	972	18	2257	81
H(10)	-955	-296	2636	63
H(11)	-2320	340	3395	66
H(12)	-1779	1307	3732	59
H(13A)	-1617	2360	3962	47
H(13B)	-843	3002	3852	47
H(14)	-1649	2507	2892	47
H(15A)	-446	3705	2839	48
H(15B)	-1180	3640	2329	48
H(17)	620	3600	899	47
H(18)	1346	4622	339	55
H(19)	2452	5274	757	57
H(20)	2742	4941	1760	61
H(21)	1991	3941	2328	53
H(23)	1531	1638	1517	61
H(24)	840	1055	860	74
H(25)	-1033	1444	614	63
H(26)	-2179	2503	977	52
H(27)	-1488	3103	1628	50
H(29)	5156	2596	4040	53
H(30)	6338	1728	4554	53
H(31)	6068	543	4646	59
H(32)	4550	227	4252	76
H(33)	3281	1111	3768	59

H(34)	2916	2688	4769	59
H(35)	1652	3414	5494	72
H(36)	110	4279	5214	67
H(37)	-117	4448	4190	62
H(38)	1171	3738	3450	52
H(40A)	3621	3679	2895	45
H(40B)	4463	3407	3383	45
H(41)	5621	2550	2671	48
H(42A)	5536	2862	1607	44
H(42B)	4361	3438	1804	44
H(44)	4006	1172	1228	56
H(45)	3857	1108	225	62
H(46)	3623	2154	-451	64
H(47)	3524	3254	-94	55
H(48)	3639	3324	918	50
H(50)	3454	913	2656	53
H(51)	4680	-186	2769	61
H(52)	6750	-290	2389	56
H(53)	7610	669	1833	67
H(54)	6399	1764	1696	65
H(89)	-5358	5775	4426	157
H(89B)	-5472	6279	4186	171
H(87)	-3930	4396	1649	81
H(87B)	-3939	4148	1399	108
H(88)	-8239	7184	2197	187
H(88B)	-8671	7534	2616	191
H(56)	-5527	8841	1768	52
H(58)	-7384	8443	544	64
H(60)	-5573	6819	1481	55
H(64)	-3151	8685	1690	55
H(66)	-194	7867	461	62
H(68)	-2597	6592	1468	46
H(72)	-2641	6564	2583	54
H(74)	-4422	4943	3486	67
H(76)	-6171	6627	2576	55
H(80)	-2917	7986	2798	46
H(82)	-5328	8908	4211	57
H(84)	-6514	8194	2865	50

Table 11. Crystal data and structure refinement for z1dppe.

Identification code	z1dppe	
Empirical formula	$C_{56}H_{54}Cl_7P_4Rh$	
Formula weight	1201.93	
Temperature	100.00(10) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.0851(4) Å	α = 88.981(3)°
	b = 12.1298(4) Å	β = 77.421(3)°
	c = 21.8397(7) Å	γ = 69.857(3)°
Volume	2685.52(16) $Å^3$	
Z	2	
Density (calculated)	1.486 Mg/m^3	
Absorption coefficient	0.823 mm^{-1}	
F(000)	1228	
Crystal size	0.407 x 0.312 x 0.209 mm^3	
Theta range for data collection	2.412 to 29.967°.	
Index ranges	-15<=h<=14, -16<=k<=16, -29<=l<=30	
Reflections collected	50653	
Independent reflections	13809 [R(int) = 0.0484]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.206	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13809 / 0 / 613	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0417, wR2 = 0.0856	
R indices (all data)	R1 = 0.0528, wR2 = 0.0920	
Largest diff. peak and hole	1.254 and -1.278 e/$Å^{-3}$	

Table 12. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for z1dppe. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	25485(2)	25957(2)	74391(2)	83(1)
P(1)	16368(6)	32399(5)	84970(3)	105(1)
P(1B)	45590(6)	28158(5)	74607(3)	95(1)
P(2)	5399(6)	24000(5)	74082(3)	104(1)
P(2B)	34676(6)	18945(5)	63837(3)	100(1)
C(1)	21740(20)	42090(20)	89317(10)	117(4)
C(1B)	51050(20)	27119(19)	82055(10)	105(4)
C(2)	20210(20)	53410(20)	87342(11)	160(5)
C(2B)	53640(20)	16340(20)	84843(11)	141(5)
C(3)	22770(20)	61510(20)	90857(12)	192(5)
C(3B)	58420(20)	14790(20)	90292(12)	181(5)
C(4)	26600(20)	58360(20)	96481(12)	201(5)
C(4B)	60590(20)	23990(20)	93035(11)	175(5)
C(5)	28170(20)	47150(20)	98498(11)	187(5)
C(5B)	58010(20)	34760(20)	90283(11)	142(5)
C(6)	25780(20)	39020(20)	94923(11)	150(5)
C(6B)	53340(20)	36290(20)	84788(10)	121(4)
C(7)	16300(20)	20610(20)	90310(11)	131(5)
C(7B)	46780(20)	42200(20)	71907(10)	139(5)
C(8)	25450(20)	9350(20)	88622(12)	172(5)
C(8B)	35230(30)	51700(20)	72096(11)	180(5)
C(9)	25690(30)	260(20)	92661(13)	243(6)
C(9B)	35540(30)	62900(20)	70906(13)	259(6)
C(10)	16740(30)	2390(30)	98434(14)	282(6)
C(10B)	47530(30)	64700(20)	69503(13)	302(7)
C(11)	7540(30)	13580(30)	100151(13)	267(6)
C(11B)	59160(30)	55230(30)	69047(13)	307(7)
C(12)	7320(30)	22600(20)	96172(12)	202(5)
C(12B)	58860(30)	44030(20)	70206(12)	216(5)
C(13)	-1040(20)	42230(20)	86791(11)	145(5)
C(13B)	60910(20)	17230(20)	70072(11)	138(5)
C(14)	-11040(20)	37190(20)	85397(11)	171(5)
C(14B)	61520(20)	15770(20)	63096(11)	159(5)

C(15)	-9850(20)	35400(20)	78383(11)	152(5)
C(15B)	52220(20)	9710(20)	61883(11)	133(5)
C(16)	230(20)	24880(20)	66576(10)	115(4)
C(16B)	29290(20)	8530(20)	60093(10)	121(4)
C(17)	-2930(20)	15960(20)	64085(11)	137(5)
C(17B)	24730(20)	10690(20)	54575(11)	152(5)
C(18)	-7110(20)	17390(20)	58440(11)	176(5)
C(18B)	21840(20)	2070(20)	51671(11)	185(5)
C(19)	-8430(20)	27620(20)	55338(12)	198(5)
C(19B)	23370(20)	-8700(20)	54269(12)	202(5)
C(20)	-5510(30)	36610(20)	57831(12)	212(5)
C(20B)	27900(20)	-10930(20)	59783(12)	199(5)
C(21)	-1140(20)	35160(20)	63411(12)	175(5)
C(21B)	30970(20)	-2410(20)	62647(11)	155(5)
C(22)	3750(20)	10340(20)	77195(11)	130(5)
C(22B)	34350(20)	30400(20)	58180(11)	138(5)
C(23)	-8380(20)	8690(20)	79024(12)	179(5)
C(23B)	41920(20)	27760(20)	52022(12)	195(5)
C(24)	-8870(30)	-2050(20)	81144(13)	243(6)
C(24B)	41900(30)	36630(30)	47927(12)	254(6)
C(25)	2630(30)	-11160(20)	81530(13)	252(6)
C(25B)	34410(30)	48230(30)	49879(13)	275(6)
C(26)	14660(30)	-9530(20)	79834(12)	226(6)
C(26B)	26870(30)	50930(20)	55984(13)	268(6)
C(27)	15190(20)	1160(20)	77672(11)	157(5)
C(27B)	26850(20)	42060(20)	60098(12)	179(5)
Cl(2)	60601(10)	83962(7)	94330(4)	443(2)
Cl(3)	52240(8)	67449(6)	88547(4)	362(2)
Cl(4)	77471(9)	69608(10)	83230(6)	777(4)
C(29)	61200(30)	77150(20)	87203(14)	281(6)
Cl(5)	97140(9)	65616(7)	68954(4)	496(2)
Cl(6)	80155(10)	72461(8)	60116(4)	489(2)
Cl(7)	91073(10)	88651(7)	64269(4)	475(2)
C(28)	84760(30)	77390(20)	66453(13)	267(6)
Cl(1)	52441(6)	91284(5)	75109(3)	183(1)

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Table 13. Bond lengths [Å] for z1dppe.

Rh(1)-P(1)	2.3394(6)	C(7)-C(8)	1.389(3)
Rh(1)-P(1B)	2.3445(6)	C(7)-C(12)	1.407(3)
Rh(1)-P(2)	2.3342(6)	C(7B)-C(8B)	1.389(3)
Rh(1)-P(2B)	2.3504(6)	C(7B)-C(12B)	1.401(3)
P(1)-C(1)	1.845(2)	C(8)-H(8)	0.9300
P(1)-C(7)	1.830(2)	C(8)-C(9)	1.396(4)
P(1)-C(13)	1.844(2)	C(8B)-H(8B)	0.9300
P(1B)-C(1B)	1.843(2)	C(8B)-C(9B)	1.389(3)
P(1B)-C(7B)	1.831(2)	C(9)-H(9)	0.9300
P(1B)-C(13B)	1.840(2)	C(9)-C(10)	1.390(4)
P(2)-C(15)	1.843(2)	C(9B)-H(9B)	0.9300
P(2)-C(16)	1.841(2)	C(9B)-C(10B)	1.389(4)
P(2)-C(22)	1.831(2)	C(10)-H(10)	0.9300
P(2B)-C(15B)	1.837(2)	C(10)-C(11)	1.386(4)
P(2B)-C(16B)	1.841(2)	C(10B)-H(10B)	0.9300
P(2B)-C(22B)	1.839(2)	C(10B)-C(11B)	1.386(4)
C(1)-C(2)	1.396(3)	C(11)-H(11)	0.9300
C(1)-C(6)	1.395(3)	C(11)-C(12)	1.381(4)
C(1B)-C(2B)	1.397(3)	C(11B)-H(11B)	0.9300
C(1B)-C(6B)	1.393(3)	C(11B)-C(12B)	1.388(4)
C(2)-H(2)	0.9300	C(12)-H(12)	0.9300
C(2)-C(3)	1.397(3)	C(12B)-H(12B)	0.9300
C(2B)-H(2B)	0.9300	C(13)-H(13A)	0.9700
C(2B)-C(3B)	1.389(3)	C(13)-H(13B)	0.9700
C(3)-H(3)	0.9300	C(13)-C(14)	1.521(3)
C(3)-C(4)	1.390(4)	C(13B)-H(13C)	0.9700
C(3B)-H(3B)	0.9300	C(13B)-H(13D)	0.9700
C(3B)-C(4B)	1.390(3)	C(13B)-C(14B)	1.521(3)
C(4)-H(4)	0.9300	C(14)-H(14A)	0.9700
C(4)-C(5)	1.387(4)	C(14)-H(14B)	0.9700
C(4B)-H(4B)	0.9300	C(14)-C(15)	1.522(3)
C(4B)-C(5B)	1.393(3)	C(14B)-H(14C)	0.9700
C(5)-H(5)	0.9300	C(14B)-H(14D)	0.9700
C(5)-C(6)	1.396(3)	C(14B)-C(15B)	1.523(3)
C(5B)-H(5B)	0.9300	C(15)-H(15A)	0.9700
C(5B)-C(6B)	1.392(3)	C(15)-H(15B)	0.9700
C(6)-H(6)	0.9300	C(15B)-H(15C)	0.9700
C(6B)-H(6B)	0.9300	C(15B)-H(15D)	0.9700

C(16)-C(17)	1.397(3)	C(26B)-H(26B)	0.9300
C(16)-C(21)	1.393(3)	C(26B)-C(27B)	1.389(4)
C(16B)-C(17B)	1.393(3)	C(27)-H(27)	0.9300
C(16B)-C(21B)	1.399(3)	C(27B)-H(27B)	0.9300
C(17)-H(17)	0.9300	Cl(2)-C(29)	1.753(3)
C(17)-C(18)	1.397(3)	Cl(3)-C(29)	1.768(3)
C(17B)-H(17B)	0.9300	Cl(4)-C(29)	1.747(3)
C(17B)-C(18B)	1.394(3)	C(29)-H(29)	0.9800
C(18)-H(18)	0.9300	Cl(5)-C(28)	1.781(3)
C(18)-C(19)	1.382(4)	Cl(6)-C(28)	1.755(3)
C(18B)-H(18B)	0.9300	Cl(7)-C(28)	1.753(3)
C(18B)-C(19B)	1.385(4)	C(28)-H(28)	0.9800
C(19)-H(19)	0.9300		
C(19)-C(20)	1.390(4)		
C(19B)-H(19B)	0.9300		
C(19B)-C(20B)	1.390(4)		
C(20)-H(20)	0.9300		
C(20)-C(21)	1.393(3)		
C(20B)-H(20B)	0.9300		
C(20B)-C(21B)	1.391(3)		
C(21)-H(21)	0.9300		
C(21B)-H(21B)	0.9300		
C(22)-C(23)	1.399(3)		
C(22)-C(27)	1.393(3)		
C(22B)-C(23B)	1.398(3)		
C(22B)-C(27B)	1.388(3)		
C(23)-H(23)	0.9300		
C(23)-C(24)	1.390(4)		
C(23B)-H(23B)	0.9300		
C(23B)-C(24B)	1.386(4)		
C(24)-H(24)	0.9300		
C(24)-C(25)	1.388(4)		
C(24B)-H(24B)	0.9300		
C(24B)-C(25B)	1.383(4)		
C(25)-H(25)	0.9300		
C(25)-C(26)	1.386(4)		
C(25B)-H(25B)	0.9300		
C(25B)-C(26B)	1.388(4)		
C(26)-H(26)	0.9300		
C(26)-C(27)	1.388(4)		

Table 14. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for z1dppe. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	76(1)	114(1)	67(1)	-4(1)	-15(1)	-43(1)
P(1)	91(3)	137(3)	86(3)	-18(2)	-13(2)	-43(2)
P(1B)	93(3)	123(3)	80(3)	1(2)	-17(2)	-51(2)
P(2)	90(3)	135(3)	90(3)	-11(2)	-18(2)	-45(2)
P(2B)	85(3)	139(3)	80(3)	-4(2)	-12(2)	-46(2)
C(1)	83(10)	172(11)	94(11)	-38(9)	-4(8)	-50(9)
C(1B)	74(10)	139(11)	101(11)	1(8)	-13(8)	-41(9)
C(2)	139(12)	199(12)	140(12)	-8(9)	-32(9)	-57(10)
C(2B)	175(12)	144(11)	133(11)	-2(9)	-48(9)	-85(9)
C(3)	180(13)	162(12)	235(13)	-24(10)	-34(10)	-68(10)
C(3B)	214(13)	174(12)	171(12)	48(9)	-74(10)	-70(10)
C(4)	203(13)	243(13)	177(13)	-67(10)	-30(10)	-108(11)
C(4B)	187(12)	242(13)	124(12)	12(9)	-77(9)	-83(10)
C(5)	168(12)	285(14)	119(12)	-35(10)	-30(9)	-90(11)
C(5B)	143(11)	197(12)	113(11)	-21(9)	-22(9)	-97(10)
C(6)	106(11)	204(12)	120(11)	-17(9)	-12(9)	-35(9)
C(6B)	112(11)	146(11)	112(11)	15(9)	-15(8)	-60(9)
C(7)	124(11)	178(12)	119(11)	15(9)	-46(9)	-78(9)
C(7B)	212(12)	183(12)	69(11)	32(9)	-48(9)	-118(10)
C(8)	134(12)	203(13)	180(13)	5(10)	-36(9)	-59(10)
C(8B)	231(13)	182(12)	118(12)	20(9)	-26(10)	-71(10)
C(9)	221(14)	217(14)	296(15)	55(11)	-91(11)	-63(11)
C(9B)	396(17)	151(13)	195(14)	26(10)	-45(12)	-67(12)
C(10)	296(16)	308(16)	300(16)	176(12)	-100(12)	-164(13)
C(10B)	600(20)	215(14)	198(14)	51(11)	-122(13)	-252(14)
C(11)	259(15)	346(16)	202(14)	73(11)	-9(11)	-140(12)
C(11B)	412(18)	426(18)	256(15)	135(13)	-139(13)	-329(15)
C(12)	192(13)	244(14)	160(13)	8(10)	-3(10)	-85(11)
C(12B)	226(14)	290(14)	201(13)	82(11)	-84(11)	-156(11)
C(13)	103(11)	179(12)	134(11)	-43(9)	-8(9)	-33(9)
C(13B)	81(11)	196(12)	124(11)	-35(9)	-6(8)	-40(9)
C(14)	117(11)	246(13)	135(12)	-56(10)	-2(9)	-58(10)
C(14B)	103(11)	244(13)	128(11)	-30(9)	6(9)	-72(10)
C(15)	95(11)	192(12)	164(12)	-35(9)	-27(9)	-45(9)
C(15B)	105(11)	163(12)	104(11)	-35(9)	2(8)	-26(9)

C(16)	74(10)	170(11)	87(11)	-10(8)	-13(8)	-29(9)
C(16B)	88(11)	157(11)	95(11)	-49(8)	13(8)	-32(9)
C(17)	112(11)	188(12)	121(11)	1(9)	-12(9)	-75(9)
C(17B)	108(11)	195(12)	124(11)	-25(9)	-19(9)	-20(9)
C(18)	115(11)	270(14)	166(12)	-53(10)	-21(9)	-99(10)
C(18B)	137(12)	290(14)	127(12)	-68(10)	-33(9)	-65(10)
C(19)	148(12)	294(14)	144(12)	11(10)	-75(10)	-42(11)
C(19B)	182(13)	224(13)	207(13)	-97(10)	-22(10)	-86(11)
C(20)	227(13)	207(13)	192(13)	49(10)	-86(10)	-41(11)
C(20B)	195(13)	189(13)	225(13)	-30(10)	-22(10)	-94(10)
C(21)	193(13)	180(12)	175(12)	12(9)	-60(10)	-82(10)
C(21B)	149(12)	206(12)	102(11)	-17(9)	-6(9)	-66(10)
C(22)	147(11)	151(11)	93(11)	-13(8)	-5(9)	-66(9)
C(22B)	131(11)	193(12)	110(11)	33(9)	-41(9)	-75(9)
C(23)	149(12)	214(13)	187(13)	31(10)	-25(10)	-89(10)
C(23B)	162(12)	245(13)	148(12)	14(10)	-6(10)	-51(10)
C(24)	248(14)	295(15)	226(14)	38(11)	-5(11)	-178(12)
C(24B)	216(14)	388(17)	146(13)	90(11)	-13(10)	-112(12)
C(25)	366(16)	179(13)	226(14)	46(10)	-38(12)	-133(12)
C(25B)	281(15)	304(15)	257(15)	155(12)	-73(12)	-123(12)
C(26)	268(14)	171(13)	207(13)	9(10)	-52(11)	-39(11)
C(26B)	324(16)	189(13)	260(15)	54(11)	-61(12)	-58(12)
C(27)	144(12)	197(12)	120(11)	-29(9)	-7(9)	-59(10)
C(27B)	191(13)	197(12)	134(12)	2(9)	-21(10)	-59(10)
Cl(2)	734(6)	388(4)	420(5)	197(4)	-338(4)	-342(4)
Cl(3)	516(5)	276(4)	375(4)	79(3)	-179(4)	-196(3)
Cl(4)	314(5)	599(7)	1003(9)	348(6)	188(5)	135(4)
C(29)	248(15)	254(15)	280(15)	111(12)	-12(12)	-42(12)
Cl(5)	515(5)	249(4)	527(5)	16(4)	15(4)	31(4)
Cl(6)	781(7)	611(6)	269(4)	-29(4)	-36(4)	-534(5)
Cl(7)	740(6)	376(4)	543(5)	153(4)	-291(5)	-402(5)
C(28)	363(16)	213(14)	220(14)	-19(11)	-1(12)	-130(12)
Cl(1)	221(3)	179(3)	156(3)	17(2)	-51(2)	-73(2)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for z1dppe.

	x	y	z	U(eq)
H(2)	1744	5558	8363	19
H(2B)	5216	1017	8304	17
H(3)	2193	6896	8945	23
H(3B)	6017	758	9211	22
H(4)	2811	6379	9889	24
H(4B)	6375	2296	9669	21
H(5)	3082	4504	10224	22
H(5B)	5940	4095	9212	17
H(6)	2688	3150	9629	18
H(6B)	5174	4346	8293	15
H(8)	3148	785	8477	21
H(8B)	2718	5054	7303	22
H(9)	3187	-724	9148	29
H(9B)	2773	6918	7105	31
H(10)	1691	-366	10113	34
H(10B)	4775	7224	6887	36
H(11)	150	1503	10400	32
H(11B)	6721	5638	6796	37
H(12)	114	3008	9738	24
H(12B)	6671	3770	6985	26
H(13A)	-353	4473	9122	17
H(13B)	-169	4920	8445	17
H(13C)	6828	1946	7054	17
H(13D)	6201	967	7187	17
H(14A)	-1986	4248	8730	20
H(14B)	-978	2970	8730	20
H(14C)	7047	1117	6095	19
H(14D)	5920	2345	6137	19
H(15A)	-1050	4282	7649	18
H(15B)	-1730	3339	7782	18
H(15C)	5343	279	6432	16
H(15D)	5467	705	5747	16

H(17)	-224	910	6618	16
H(17B)	2361	1792	5282	18
H(18)	-902	1137	5675	21
H(18B)	1886	355	4797	22
H(19)	-1127	2849	5159	24
H(19B)	2138	-1441	5233	24
H(20)	-646	4355	5579	25
H(20B)	2887	-1813	6156	24
H(21)	89	4116	6505	21
H(21B)	3417	-400	6629	19
H(23)	-1612	1480	7882	21
H(23B)	4702	2000	5066	23
H(24)	-1695	-314	8231	29
H(24B)	4694	3476	4384	30
H(25)	225	-1835	8293	30
H(25B)	3444	5417	4713	33
H(26)	2237	-1559	8014	27
H(26B)	2179	5871	5733	32
H(27)	2330	220	7653	19
H(27B)	2177	4396	6418	21
H(29)	5708	8326	8455	34
H(28)	7702	8038	6995	32