SUPPORTING INFORMATION

Preparation of Metal-Imidazolidin-2-ylidene Complexes by Oxidative Addition

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Thiourea 5. Thiophosgene (0.30 mL, 3.54 mmol) is slowly added to a solution of diamine **4** (1.0 g, 3.54 mmol) in CH_2Cl_2 (10 mL) and Et_3N (1 mL) and the resulting mixture is stirred for 3 h at ambient temperature under argon. For work-up, the mixture is diluted with CH_2Cl_2 (30 mL) and the reaction is quenched with water. The aqueous phase is repeatedly extracted with CH_2Cl_2, the combined organic layers are dried (Na_2SO_4), the solvent is evaporated and the residue is purified by flash chromatography (hexanes/ethyl acetate, 50:1) to give thiourea **5** as a colorless solid (739 mg, 64%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 3.64 (ddd, J = 13.5, 9.8, 7.2 Hz, 2H), 3.47 (ddd, J = 17.1, 9.1, 7.9 Hz, 2H), 2.83-2.85 (m, 2H), 2.07-2.09 (m, 2H), 1.85-1.87 (m, 2H), 1.34-1.41 (m, 8H), 0.93 (s, 18H). ^{13}C NMR (100 MHz, CD_2Cl_2): δ 185.7, 64.5, 41.9, 39.7, 29.7, 29.1, 28.5, 24.4. IR (KBr): 3000, 2865, 1453, 1412, 1378, 1365, 1350, 1340, 1320, 1257, 1234, 1203, 1169, 1135, 1113, 1066, 1023, 968, 913, 834, 776, 747, 658, 627, 551, 486. MS (EI) *m/z*: 324, 309, 291, 267, 253, 239, 207, 183, 169, 155, 124, 110, 95, 81, 69, 57, 44. HRMS: *calcd.* ($C_{19}H_{36}N_2S$): 324.2599; *found* 324.2600. Anal. *calcd.* C 70.31, H 11.18, N 8.63; *found* C 70.15, H 11.03, N 8.48.

Imidazolium Chloride 6. Oxalyl chloride (0.18 mL, 2.12 mmol) is added to a solution of thiourea **5** (575 mg, 1.77 mmol) in toluene. The resulting bright yellow solution is stirred for 8 h at 60 °C under argon, causing the precipitation of a pale brown solid. This precipitate is allowed to settle, the solution was siphoned off, and the solid is repeatedly triturated with Et_2O to give salt **6** as a colorless solid (529 mg, 82%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 3.91-3.94 (m, 2H), 3.54-3.68 (m, 4H), 2.23-2.26 (m, 2H), 1.92-1.97 (m, 2H), 1.66-1.75 (m, 2H), 1.56 (ddd, J = 13.0, 11.4, 6.3 Hz, 2H), 1.38-1.50 (m, 4H), 0.96 (s, 18H). ^{13}C NMR (100 MHz, CD_2Cl_2): δ 158.1, 67.9, 43.7, 41.2, 29.9, 28.9, 27.5, 23.7. IR (KBr): 3000, 2868, 1578, 1466, 1419, 1383, 1366, 1328, 1309, 1269, 1250, 1176, 1112, 1065, 1022, 966, 912, 834, 757, 645, 518. MS (ESI-pos.) *m/z*: 327.3 ($[M-Cl]^+$). Anal. *calcd.* C 62.80, H 9.98, N 7.71; *found* C 62.63, H 9.98, N 7.74.

Representative Procedure for the Oxidative Insertion Reactions. Preparation of Complex *trans*-2a. A solution of the imidazolinum salt **1a** (128 mg, 0.46 mmol) and $Pd(PPh_3)_4$ (526 mg, 0.46 mmol) in anhydrous CH_2Cl_2 (30 mL) is refluxed under Ar for 6h. The solvent is removed in vacuo, the waxy residue is suspended in pentane and stirred for 1 h to form a fine powder. The pentane is discarded and the residue is extracted with pentane to remove the remaining PPh_3. Recrystallization of the crude product from the minimum amount of $CHCl_3$ (ca. 3 mL) affords complex **2a** as a white solid (302 mg, 72%). Eventually, it may be necessary to induce crystallization by slowly diffusing pentane into the $CHCl_3$ solution. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.70-7.60 (m, 12H), 7.60-7.40 (m, 18H), 2.84 (s, 6H), 2.64 (s, 4H); ^{13}C NMR (75 MHz, CD_2Cl_2): δ 194.9 (J_{P-C} = 6.9 Hz), 134.5 ($|^2J_{P-C} + {}^4J_{P-C}|$ = 12.6 Hz), 132.4, 129.4 ($|^3J_{P-C} + {}^5J_{P-C}|$ = 10.8 Hz), 129.0 ($|^1J_{P-C} + {}^3J_{P-C}|$ = 51.2 Hz), 51.0, 37.0; ^{31}P NMR (121 Hz, CD_2Cl_2): δ 22.5, -143.9 (hept., J_{PF} = 710 Hz).

All other complexes were obtained analogously:

Complex *trans*-2b. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.60-7.70 (m, 12H), 7.50-7.60 (m, 18H), 2.84 (s, 6H), 2.68 (s, 4H). ^{13}C NMR (75 MHz, CD_2Cl_2): δ 194.7 (J_{P-C} = 6.9 Hz), 134.6 ($|^2J_{P-C} + {}^4J_{P-C}|$ = 12.6 Hz), 132.4, 129.4 ($|^3J_{P-C} + {}^5J_{P-C}|$ = 10.8 Hz), 129.0 ($|^1J_{P-C} + {}^3J_{P-C}|$ = 51 Hz), 51.1, 37.0. ^{31}P NMR (162 Hz, CD_2Cl_2): δ 22.8.

Complex *trans*-2c. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.66-7.73 (m, 12H), 7.56-7.61 (m, 18H), 2.86 (s, 6H), 2.77 (s, 4H). ^{13}C NMR (75 MHz, CD_2Cl_2): δ 194.2 ($J_{P\text{-}C}$ = 6.9 Hz), 134.6 ($|^{2}J_{P\text{-}C} + {}^{4}J_{P\text{-}C}|$ = 12.8 Hz), 132.4, 129.5 ($|^{3}J_{P\text{-}C} + {}^{5}J_{P\text{-}C}|$ = 10.5 Hz), 51.3, 37.1. ^{31}P NMR (162 Hz, CD_2Cl_2): δ 22.5. Anal. *calcd.* for $C_{41}H_{40}Cl_2N_2P_2Pd$: C 61.55, H 5.04, N 3.50; *found* C 61.76, H 4.99, N 3.32.

Complex 7. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.71-7.76 (m, 6H), 7.47-7.52 (m, 3H), 7.39-7.44 (m, 6H), 4.03 (dt, J = 13.2, 4.7 Hz, 1H), 3.90 (dt, J = 13.4, 4.4 Hz, 1H), 3.43 (dt, J = 13.1, 4.8 Hz), 3.01 (dt, J = 13.1, 4.7 Hz, 1H), 2.88-2.95 (m, 1H), 1.93-2.01 (m, 2H), 1.83-1.92 (m, 2H), 1.69-1.82 (m, 3H), 0.98-1.37 (m, 6H), 0.93 (s, 9H), 0.92 (s, 9H). ^{13}C NMR (100 MHz, CD_2Cl_2): δ 194.5, 134.9 ($|^{2}J_{P\text{-}C} + {}^{4}J_{P\text{-}C}|$ = 11.2 Hz), 131.3 (J = 2.7 Hz), 130.9 ($|^{1}J_{P\text{-}C} + {}^{3}J_{P\text{-}C}|$ = 52.9 Hz), 128.5 ($|^{3}J_{P\text{-}C} + {}^{5}J_{P\text{-}C}|$ = 11.0 Hz), 67.8, 67.2, 45.9, 45.3, 42.2, 39.9, 29.8, 29.7, 29.1, 28.9, 28.0, 24.0, 23.8. ^{31}P NMR (162 Hz, CD_2Cl_2): δ 27.5. IR (KBr): 3054, 2952, 2865, 1587, 1573, 1483, 1450, 1436, 1394, 1365, 1354, 1325, 1307, 1251, 1236, 1191, 1162, 1095, 1064, 1028, 999, 967, 911, 842, 749, 695, 662, 641, 616, 533, 513, 494. MS (ESI-pos) *m/z*: 695.25 ($[M\text{-}Cl]^{+}$).

Crystal Structure Determinations

Crystal structure determinations for $[(C_5H_{10}N_2)Pd(PPh_3)_2Cl]^+ Cl^- \cdot 7CHCl_3$ and $(C_5H_{10}N_2)PdPPh_3Cl_2 \cdot 1.5THF$ were carried out using a Bruker-Nonius FR591 rotating anode generator equipped with a molybdenum target and a 0.3 by 3 mm filament. The crystal was mounted in a small amount of inert perfluoropolyether (Lancaster) at the end of a thin glass fiber. A Bruker-Nonius Mach3 goniostat was used to orient the crystal in the X-ray beam and diffracted intensities were recorded using a Bruker-Nonius KappaCCD area detector. Unit cell data were obtained from a combination of phi and phi-chi scans using the program DIRAX for indexing.[1] The program collect (Bruker Nonius B. V., Delft, The Netherlands) was employed to calculate a data collection strategy, based on a crystal detector distance of 40 mm and a required completeness exceeding 95 % in the range up to 66° Bragg angle. The redundancy of the reflection data was specified to lie between 2 and 6. Reflection intensities were collected using a scan speed of 0.1° per minute for $(C_5H_{10}N_2)PdPPh_3Cl_2 \cdot 1.5$ THF and 0.2° per minute for $[(C_5H_{10}N_2)Pd(PPh_3)_2Cl]^+ Cl^- \cdot 7$ $CHCl_3$. These data frames were subsequently analysed using the DENZO suite of programs.[2] All crystal faces were indexed for subsequent absorption correction using the Gaussian method as implemented in XPREP (Bruker AXS Inc., Madison, USA).

Crystal structure solution for both compounds was achieved using direct methods as implemented in SHELXS-97 (Sheldrick, G. M., program for crystal structure determination, Universität Göttingen, Germany, 1997) and visualised using the XP program (Bruker AXS Inc., Madison, USA). Missing atoms were subsequently located from difference Fourier synthesis and added to the atom list. Least-squares refinement based on F^2 using all measured intensities was carried out using the program SHELXL-97 (Sheldrick, G. M., program for crystal structure least-squares refinement, Universität Göttingen, Germany, 1997). All non-hydrogen atoms were refined including anisotropic displacement parameters. Hydrogen atoms were invariably placed in geometrically optimised positions and forced to ride on the atom to which they are attached.

For $(C_5H_{10}N_2)PdPPh_3Cl_2 \cdot 1.5$ THF one molecule of THF is situated on a crystallographic two-fold axis passing through the oxygen O(91) and the midpoint of the bond C(93)-C(93)*.

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[1] Duisenberg, A. J. M. *J. Appl. Crystallogr.* **1992**, *25*, 92-96.
[2] Otwinowski, Z.; Minor, W. *Methods Enzymol.* **1997**, *276*, 307-326.

Table 1. Complex 3: Crystal data and structure refinement $(C_5H_{10}N_2)PdPPh_3Cl_2 \cdot 1.5$ THF.

Empirical formula	$C_{29}H_{37}Cl_2N_2O_{1.50}PPd$	
Color	colorless	
Formula weight	645.88 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	**Pbcn, (no. 60)**	
Unit cell dimensions	a = 28.9418(10) Å	α= 90°.
	b = 17.7340(6) Å	β= 90°.
	c = 11.2349(3) Å	γ = 90°.
Volume	5766.4(3) Å^3	
Z	8	
Density (calculated)	1.488 Mg · m^{-3}	
Absorption coefficient	0.912 mm^{-1}	
F(000)	2656 e	
Crystal size	0.08 x 0.04 x 0.02 mm^3	
θ range for data collection	4.58 to 27.49°.	
Index ranges	$-37 \le h \le 28$, $-23 \le k \le 17$, $-13 \le l \le 14$	
Reflections collected	39321	
Independent reflections	6580 [R_{int} = 0.2058]	
Reflections with I>2σ(I)	3985	
Completeness to θ = 25.00°	99.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6580 / 0 / 333	
Goodness-of-fit on F^2	1.098	
Final R indices [I>2σ(I)]	R_1 = 0.0937	wR^2 = 0.1721
R indices (all data)	R_1 = 0.1641	wR^2 = 0.1981
Extinction coefficient	0.0033(3)	
Largest diff. peak and hole	1.425 and -0.948 e · Å^{-3}	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for Complex 3 [$(C_5H_{10}N_2)PdPPh_3Cl_2 \cdot$ 1.5 THF]. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Pd(1)	0.2853(1)	0.2481(1)	0.1036(1)	0.016(1)
Cl(1)	0.2091(1)	0.2022(1)	0.1153(2)	0.023(1)
Cl(2)	0.3197(1)	0.1270(1)	0.1067(2)	0.021(1)
P(1)	0.3572(1)	0.2961(1)	0.0920(2)	0.016(1)
N(1)	0.2455(2)	0.3898(3)	0.0119(5)	0.018(1)
N(2)	0.2458(2)	0.3867(3)	0.2062(5)	0.016(1)
C(1)	0.2573(3)	0.3492(4)	0.1071(7)	0.019(2)
C(2)	0.2563(3)	0.3701(5)	-0.1100(7)	0.024(2)
C(3)	0.2292(3)	0.4657(5)	0.0439(7)	0.023(2)
C(4)	0.2224(3)	0.4579(5)	0.1783(7)	0.028(2)
C(5)	0.2512(3)	0.3614(5)	0.3265(7)	0.025(2)
C(11)	0.3904(3)	0.2477(5)	-0.0213(6)	0.020(2)
C(12)	0.3705(3)	0.2413(5)	-0.1358(7)	0.025(2)
C(13)	0.3930(3)	0.2040(5)	-0.2256(7)	0.028(2)
C(14)	0.4363(3)	0.1724(5)	-0.2058(7)	0.026(2)
C(15)	0.4565(3)	0.1785(5)	-0.0951(7)	0.028(2)
C(16)	0.4335(3)	0.2161(5)	-0.0032(7)	0.024(2)
C(21)	0.3632(3)	0.3957(4)	0.0579(7)	0.018(2)
C(22)	0.3468(3)	0.4485(4)	0.1399(7)	0.021(2)
C(23)	0.3493(3)	0.5261(5)	0.1155(8)	0.029(2)
C(24)	0.3670(3)	0.5511(5)	0.0101(8)	0.028(2)
C(25)	0.3849(3)	0.5000(5)	-0.0727(7)	0.029(2)
C(26)	0.3827(3)	0.4224(5)	-0.0497(7)	0.025(2)
C(31)	0.3884(3)	0.2862(4)	0.2334(6)	0.018(2)
C(32)	0.3706(3)	0.2386(5)	0.3194(7)	0.023(2)
C(33)	0.3943(3)	0.2322(4)	0.4283(7)	0.029(2)
C(34)	0.4347(3)	0.2710(5)	0.4483(8)	0.028(2)
C(35)	0.4514(3)	0.3195(5)	0.3635(8)	0.028(2)
C(36)	0.4279(3)	0.3277(5)	0.2553(7)	0.021(2)
O(91)	0.5000	0.4884(8)	0.2500	0.107(6)
C(92)	0.4852(5)	0.5270(10)	0.1626(13)	0.082(5)
C(93)	0.4874(4)	0.6086(8)	0.1924(14)	0.088(6)
O(95)	0.4442(2)	0.0728(3)	0.5088(5)	0.029(1)
C(96)	0.4669(3)	0.0667(6)	0.3951(8)	0.041(2)
C(97)	0.4307(3)	0.0458(5)	0.3043(8)	0.035(2)
C(98)	0.3888(3)	0.0225(5)	0.3793(8)	0.034(2)
C(99)	0.4080(3)	0.0191(5)	0.5072(8)	0.032(2)

Table 3. Bond lengths [Å] and angles [°] for Complex 3 [$(C_5H_{10}N_2)PdPPh_3Cl_2 \cdot 1.5$ THF].

Pd(1)-C(1)	1.968(8)	Pd(1)-P(1)	2.251(2)
Pd(1)-Cl(1)	2.355(2)	Pd(1)-Cl(2)	2.3676(19)
P(1)-C(11)	1.810(8)	P(1)-C(21)	1.816(8)
P(1)-C(31)	1.835(8)	N(1)-C(1)	1.334(9)
N(1)-C(2)	1.448(10)	N(1)-C(3)	1.471(10)
N(2)-C(1)	1.339(10)	N(2)-C(5)	1.433(9)
N(2)-C(4)	1.467(10)	C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800	C(2)-H(2C)	0.9800
C(3)-C(4)	1.529(11)	C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900	C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900	C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800	C(5)-H(5C)	0.9800
C(11)-C(16)	1.384(11)	C(11)-C(12)	1.414(10)
C(12)-C(13)	1.371(11)	C(12)-H(12)	0.9500
C(13)-C(14)	1.391(12)	C(13)-H(13)	0.9500
C(14)-C(15)	1.378(11)	C(14)-H(14)	0.9500
C(15)-C(16)	1.396(11)	C(15)-H(15)	0.9500
C(16)-H(16)	0.9500	C(21)-C(22)	1.398(11)
C(21)-C(26)	1.416(10)	C(22)-C(23)	1.405(11)
C(22)-H(22)	0.9500	C(23)-C(24)	1.363(12)
C(23)-H(23)	0.9500	C(24)-C(25)	1.398(12)
C(24)-H(24)	0.9500	C(25)-C(26)	1.403(12)
C(25)-H(25)	0.9500	C(26)-H(26)	0.9500
C(31)-C(36)	1.382(11)	C(31)-C(32)	1.383(11)
C(32)-C(33)	1.407(11)	C(32)-H(32)	0.9500
C(33)-C(34)	1.376(13)	C(33)-H(33)	0.9500
C(34)-C(35)	1.371(12)	C(34)-H(34)	0.9500
C(35)-C(36)	1.400(11)	C(35)-H(35)	0.9500
C(36)-H(36)	0.9500	O(91)-C(92)	1.271(18)
O(91)-C(92)*	1.271(18)	C(92)-C(93)	1.487(19)
C(92)-H(92A)	0.9900	C(92)-H(92B)	0.9900
C(93)-C(93)*	1.49(3)	C(93)-H(93A)	0.9900
C(93)-H(93B)	0.9900	O(95)-C(99)	1.416(10)
O(95)-C(96)	1.440(10)	C(96)-C(97)	1.508(12)
C(96)-H(96A)	0.9900	C(96)-H(96B)	0.9900
C(97)-C(98)	1.534(13)	C(97)-H(97A)	0.9900
C(97)-H(97B)	0.9900	C(98)-C(99)	1.541(12)
C(98)-H(98A)	0.9900	C(98)-H(98B)	0.9900

C(99)-H(99A)	0.9900	C(99)-H(99B)	0.9900
C(1)-Pd(1)-P(1)	92.2(2)	C(1)-Pd(1)-Cl(1)	85.9(2)
P(1)-Pd(1)-Cl(1)	178.04(8)	C(1)-Pd(1)-Cl(2)	178.0(2)
P(1)-Pd(1)-Cl(2)	87.46(7)	Cl(1)-Pd(1)-Cl(2)	94.50(7)
C(11)-P(1)-C(21)	105.2(4)	C(11)-P(1)-C(31)	107.6(4)
C(21)-P(1)-C(31)	103.2(4)	C(11)-P(1)-Pd(1)	110.6(3)
C(21)-P(1)-Pd(1)	117.9(3)	C(31)-P(1)-Pd(1)	111.6(3)
C(1)-N(1)-C(2)	124.9(7)	C(1)-N(1)-C(3)	112.4(6)
C(2)-N(1)-C(3)	121.5(6)	C(1)-N(2)-C(5)	127.0(6)
C(1)-N(2)-C(4)	111.4(6)	C(5)-N(2)-C(4)	121.4(6)
N(1)-C(1)-N(2)	109.5(6)	N(1)-C(1)-Pd(1)	125.6(6)
N(2)-C(1)-Pd(1)	124.9(6)	N(1)-C(2)-H(2A)	109.5
N(1)-C(2)-H(2B)	109.5	H(2A)-C(2)-H(2B)	109.5
N(1)-C(2)-H(2C)	109.5	H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5	N(1)-C(3)-C(4)	101.5(6)
N(1)-C(3)-H(3A)	111.5	C(4)-C(3)-H(3A)	111.5
N(1)-C(3)-H(3B)	111.5	C(4)-C(3)-H(3B)	111.5
H(3A)-C(3)-H(3B)	109.3	N(2)-C(4)-C(3)	103.3(6)
N(2)-C(4)-H(4A)	111.1	C(3)-C(4)-H(4A)	111.1
N(2)-C(4)-H(4B)	111.1	C(3)-C(4)-H(4B)	111.1
H(4A)-C(4)-H(4B)	109.1	N(2)-C(5)-H(5A)	109.5
N(2)-C(5)-H(5B)	109.5	H(5A)-C(5)-H(5B)	109.5
N(2)-C(5)-H(5C)	109.5	H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5	C(16)-C(11)-C(12)	117.9(7)
C(16)-C(11)-P(1)	124.6(6)	C(12)-C(11)-P(1)	117.5(6)
C(13)-C(12)-C(11)	121.0(8)	C(13)-C(12)-H(12)	119.5
C(11)-C(12)-H(12)	119.5	C(12)-C(13)-C(14)	120.3(8)
C(12)-C(13)-H(13)	119.8	C(14)-C(13)-H(13)	119.8
C(15)-C(14)-C(13)	119.6(8)	C(15)-C(14)-H(14)	120.2
C(13)-C(14)-H(14)	120.2	C(14)-C(15)-C(16)	120.3(8)
C(14)-C(15)-H(15)	119.9	C(16)-C(15)-H(15)	119.9
C(11)-C(16)-C(15)	120.9(8)	C(11)-C(16)-H(16)	119.6
C(15)-C(16)-H(16)	119.6	C(22)-C(21)-C(26)	118.3(7)
C(22)-C(21)-P(1)	118.8(6)	C(26)-C(21)-P(1)	122.9(6)
C(21)-C(22)-C(23)	120.7(7)	C(21)-C(22)-H(22)	119.7
C(23)-C(22)-H(22)	119.7	C(24)-C(23)-C(22)	120.5(8)
C(24)-C(23)-H(23)	119.7	C(22)-C(23)-H(23)	119.7
C(23)-C(24)-C(25)	120.4(8)	C(23)-C(24)-H(24)	119.8
C(25)-C(24)-H(24)	119.8	C(24)-C(25)-C(26)	119.8(8)
C(24)-C(25)-H(25)	120.1	C(26)-C(25)-H(25)	120.1

C(25)-C(26)-C(21)	120.2(8)	C(25)-C(26)-H(26)	119.9
C(21)-C(26)-H(26)	119.9	C(36)-C(31)-C(32)	120.6(7)
C(36)-C(31)-P(1)	120.7(6)	C(32)-C(31)-P(1)	118.6(6)
C(31)-C(32)-C(33)	118.3(8)	C(31)-C(32)-H(32)	120.8
C(33)-C(32)-H(32)	120.8	C(34)-C(33)-C(32)	121.1(8)
C(34)-C(33)-H(33)	119.5	C(32)-C(33)-H(33)	119.5
C(35)-C(34)-C(33)	119.9(8)	C(35)-C(34)-H(34)	120.0
C(33)-C(34)-H(34)	120.0	C(34)-C(35)-C(36)	119.9(8)
C(34)-C(35)-H(35)	120.0	C(36)-C(35)-H(35)	120.0
C(31)-C(36)-C(35)	120.0(8)	C(31)-C(36)-H(36)	120.0
C(35)-C(36)-H(36)	120.0	C(92)-O(91)-C(92)*	114.8(16)
O(91)-C(92)-C(93)	109.6(12)	O(91)-C(92)-H(92A)	109.7
C(93)-C(92)-H(92A)	109.7	O(91)-C(92)-H(92B)	109.7
C(93)-C(92)-H(92B)	109.7	H(92A)-C(92)-H(92B)	108.2
C(93)*-C(93)-C(92)	102.5(8)	C(93)*-C(93)-H(93A)	111.3
C(92)-C(93)-H(93A)	111.3	C(93)*-C(93)-H(93B)	111.3
C(92)-C(93)-H(93B)	111.3	H(93A)-C(93)-H(93B)	109.2
C(99)-O(95)-C(96)	106.0(7)	O(95)-C(96)-C(97)	107.5(7)
O(95)-C(96)-H(96A)	110.2	C(97)-C(96)-H(96A)	110.2
O(95)-C(96)-H(96B)	110.2	C(97)-C(96)-H(96B)	110.2
H(96A)-C(96)-H(96B)	108.5	C(96)-C(97)-C(98)	104.1(7)
C(96)-C(97)-H(97A)	110.9	C(98)-C(97)-H(97A)	110.9
C(96)-C(97)-H(97B)	110.9	C(98)-C(97)-H(97B)	110.9
H(97A)-C(97)-H(97B)	108.9	C(97)-C(98)-C(99)	103.7(7)
C(97)-C(98)-H(98A)	111.0	C(99)-C(98)-H(98A)	111.0
C(97)-C(98)-H(98B)	111.0	C(99)-C(98)-H(98B)	111.0
H(98A)-C(98)-H(98B)	109.0	O(95)-C(99)-C(98)	104.6(7)
O(95)-C(99)-H(99A)	110.8	C(98)-C(99)-H(99A)	110.8
O(95)-C(99)-H(99B)	110.8	C(98)-C(99)-H(99B)	110.8
H(99A)-C(99)-H(99B)	108.9		

Symmetry transformations used to generate equivalent atoms: * -x+1,y,-z+1/2

Table 4. Anisotropic displacement parameters ($Å^2$) for Complex 3 [$(C_5H_{10}N_2)PdPPh_3Cl_2 \cdot 1.5$ THF].

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}
Pd(1)	0.021(1)	0.016(1)	0.010(1)	0.000(1)	0.001(1)	0.000(1)
Cl(1)	0.022(1)	0.029(1)	0.019(1)	0.002(1)	0.002(1)	-0.004(1)
Cl(2)	0.029(1)	0.016(1)	0.017(1)	0.001(1)	-0.001(1)	0.002(1)
P(1)	0.021(1)	0.019(1)	0.008(1)	-0.001(1)	0.001(1)	0.000(1)
N(1)	0.029(4)	0.020(3)	0.006(3)	-0.004(2)	0.002(3)	0.004(3)
N(2)	0.025(4)	0.011(3)	0.014(3)	-0.002(2)	0.009(3)	0.010(3)
C(1)	0.018(4)	0.019(4)	0.020(4)	0.006(3)	0.000(3)	-0.006(3)
C(2)	0.030(5)	0.028(4)	0.016(4)	0.002(4)	-0.005(4)	0.005(4)
C(3)	0.030(5)	0.019(4)	0.021(4)	-0.004(3)	-0.002(3)	0.002(4)
C(4)	0.035(5)	0.025(5)	0.023(5)	-0.007(4)	0.007(4)	0.007(4)
C(5)	0.037(5)	0.029(5)	0.009(4)	0.006(3)	0.003(4)	0.004(4)
C(11)	0.022(4)	0.022(4)	0.017(4)	-0.006(4)	-0.001(3)	0.000(4)
C(12)	0.035(5)	0.024(5)	0.015(4)	0.000(3)	-0.003(3)	-0.004(4)
C(13)	0.045(6)	0.030(5)	0.008(4)	-0.006(3)	0.000(4)	-0.005(4)
C(14)	0.021(5)	0.036(5)	0.020(4)	-0.004(4)	0.004(3)	0.003(4)
C(15)	0.031(5)	0.034(5)	0.019(4)	0.002(4)	0.005(4)	0.006(4)
C(16)	0.033(5)	0.022(4)	0.017(4)	-0.002(3)	0.000(4)	0.005(4)
C(21)	0.020(4)	0.020(4)	0.012(4)	-0.001(3)	-0.004(3)	-0.001(3)
C(22)	0.026(5)	0.023(4)	0.013(4)	0.004(3)	0.002(3)	-0.003(4)
C(23)	0.029(5)	0.022(4)	0.034(5)	-0.007(4)	0.012(4)	-0.002(4)
C(24)	0.033(5)	0.022(4)	0.028(5)	0.003(4)	-0.008(4)	-0.003(4)
C(25)	0.049(6)	0.028(5)	0.010(4)	0.008(3)	0.003(4)	-0.004(5)
C(26)	0.036(5)	0.026(5)	0.014(4)	0.001(3)	0.007(4)	-0.002(4)
C(31)	0.026(4)	0.022(4)	0.005(4)	-0.006(3)	0.004(3)	0.004(4)
C(32)	0.025(4)	0.032(5)	0.011(4)	0.003(3)	-0.001(3)	0.002(4)
C(33)	0.058(6)	0.018(4)	0.010(4)	0.005(3)	-0.002(4)	-0.001(4)
C(34)	0.028(5)	0.037(5)	0.018(4)	-0.007(4)	-0.007(4)	0.000(4)
C(35)	0.020(5)	0.037(5)	0.026(5)	-0.006(4)	0.002(3)	0.000(4)
C(36)	0.021(4)	0.024(5)	0.017(4)	0.001(3)	0.000(3)	0.002(4)
O(91)	0.151(16)	0.054(9)	0.117(16)	0.000	-0.030(13)	0.000
C(92)	0.064(9)	0.120(14)	0.062(10)	-0.062(10)	-0.024(7)	0.000(9)
C(93)	0.046(8)	0.104(11)	0.115(14)	0.082(10)	0.002(8)	0.011(8)
O(95)	0.029(3)	0.035(3)	0.023(3)	-0.005(3)	0.000(3)	-0.008(3)

C(96)	0.039(6)	0.061(7)	0.024(5)	-0.007(5)	0.002(4)	-0.007(5)
C(97)	0.051(6)	0.039(6)	0.016(4)	-0.004(4)	-0.003(4)	-0.011(5)
C(98)	0.034(5)	0.040(5)	0.027(5)	0.004(4)	-0.007(4)	-0.004(4)
C(99)	0.032(5)	0.043(6)	0.020(5)	0.006(4)	-0.005(4)	-0.007(4)

Table 5. Crystal data and structure refinement for complex *trans*-2c $[(C_5H_{10}N_2)Pd(PPh_3)_2Cl]^+ Cl^- \cdot 7\ CHCl_3$.

Empirical formula	$C_{48} H_{47} Cl_{23} N_2 P_2 Pd$	
Color	colorless	
Formula weight	1635.57 $g \cdot mol^{-1}$	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	**$P\bar{1}$, (no. 2)**	
Unit cell dimensions	a = 14.4426(3) Å	α= 90.7160(10)°.
	b = 14.6316(3) Å	β= 98.3380(10)°.
	c = 16.3023(4) Å	γ = 94.8700(10)°.
Volume	3395.18(13) $Å^3$	
Z	2	
Density (calculated)	1.600 $Mg \cdot m^{-3}$	
Absorption coefficient	1.260 mm^{-1}	
F(000)	1632 e	
Crystal size	0.15 x 0.12 x 0.06 mm^3	
θ range for data collection	4.09 to 33.13°.	
Index ranges	$-22 \le h \le 22, -19 \le k \le 22, -25 \le l \le 18$	
Reflections collected	40763	
Independent reflections	25295 [R_{int} = 0.0429]	
Reflections with I>2σ(I)	18895	
Completeness to θ = 27.50°	98.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.93 and 0.83	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	25295 / 0 / 720	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2σ(I)]	R_1 = 0.0667	wR^2 = 0.1547
R indices (all data)	R_1 = 0.0964	wR^2 = 0.1750
Largest diff. peak and hole	2.815 and -1.834 e · $Å^{-3}$	

Table 6. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for complex *trans*-2c $[(C_5H_{10}N_2)Pd(PPh_3)_2Cl]^+ Cl^- \cdot 7\ CHCl_3$.

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Pd(1)	0.4065(1)	0.3404(1)	0.3280(1)	0.016(1)
Cl(1)	0.3728(1)	0.4183(1)	0.4460(1)	0.021(1)
Cl(2)	0.7693(1)	0.1638(1)	0.1599(1)	0.025(1)
P(1)	0.4487(1)	0.2166(1)	0.4104(1)	0.018(1)
P(2)	0.3602(1)	0.4573(1)	0.2377(1)	0.017(1)
N(1)	0.5248(2)	0.2811(2)	0.2092(2)	0.021(1)
N(2)	0.3830(2)	0.2141(2)	0.1823(2)	0.019(1)
C(1)	0.4404(2)	0.2736(2)	0.2322(2)	0.017(1)
C(2)	0.5293(2)	0.2238(2)	0.1350(2)	0.024(1)
C(3)	0.4310(3)	0.1730(2)	0.1195(2)	0.024(1)
C(4)	0.2861(2)	0.1866(2)	0.1880(2)	0.024(1)
C(5)	0.6060(2)	0.3398(3)	0.2481(2)	0.027(1)
C(11)	0.4707(2)	0.1148(2)	0.3538(2)	0.021(1)
C(12)	0.4019(3)	0.0413(2)	0.3349(2)	0.025(1)
C(13)	0.4192(3)	-0.0325(2)	0.2861(2)	0.031(1)
C(14)	0.5042(3)	-0.0337(3)	0.2560(2)	0.033(1)
C(15)	0.5724(3)	0.0387(3)	0.2740(2)	0.031(1)
C(16)	0.5561(3)	0.1126(2)	0.3231(2)	0.026(1)
C(21)	0.5549(2)	0.2387(2)	0.4848(2)	0.020(1)
C(22)	0.6012(3)	0.1660(2)	0.5216(2)	0.028(1)
C(23)	0.6816(3)	0.1830(3)	0.5787(3)	0.033(1)
C(24)	0.7181(3)	0.2730(3)	0.5997(3)	0.033(1)
C(25)	0.6727(3)	0.3455(3)	0.5620(2)	0.029(1)
C(26)	0.5922(3)	0.3287(2)	0.5053(2)	0.024(1)
C(31)	0.3527(2)	0.1773(2)	0.4656(2)	0.021(1)
C(32)	0.3655(3)	0.1165(3)	0.5310(2)	0.032(1)
C(33)	0.2890(3)	0.0828(4)	0.5668(3)	0.044(1)
C(34)	0.1999(3)	0.1105(4)	0.5401(3)	0.041(1)
C(35)	0.1872(3)	0.1716(3)	0.4769(3)	0.034(1)
C(36)	0.2630(3)	0.2040(2)	0.4393(2)	0.026(1)
C(41)	0.3489(2)	0.4252(2)	0.1277(2)	0.020(1)
C(42)	0.4275(3)	0.4261(2)	0.0873(2)	0.024(1)
C(43)	0.4187(3)	0.3946(3)	0.0054(2)	0.030(1)

C(44)	0.3316(3)	0.3615(3)	-0.0369(2)	0.033(1)
C(45)	0.2531(3)	0.3604(3)	0.0029(2)	0.033(1)
C(46)	0.2613(3)	0.3925(2)	0.0843(2)	0.027(1)
C(51)	0.4437(2)	0.5581(2)	0.2507(2)	0.019(1)
C(52)	0.4503(2)	0.6204(2)	0.1868(2)	0.022(1)
C(53)	0.5126(3)	0.6987(2)	0.1994(2)	0.026(1)
C(54)	0.5675(3)	0.7164(2)	0.2754(2)	0.027(1)
C(55)	0.5611(3)	0.6557(2)	0.3399(2)	0.026(1)
C(56)	0.4998(2)	0.5766(2)	0.3275(2)	0.023(1)
C(61)	0.2460(2)	0.4977(2)	0.2472(2)	0.021(1)
C(62)	0.1878(3)	0.4552(3)	0.2981(3)	0.033(1)
C(63)	0.0998(3)	0.4865(4)	0.3025(3)	0.044(1)
C(64)	0.0701(3)	0.5593(3)	0.2563(3)	0.037(1)
C(65)	0.1275(3)	0.6011(3)	0.2045(3)	0.040(1)
C(66)	0.2151(3)	0.5713(3)	0.2000(3)	0.034(1)
C(10)	0.3093(3)	0.8745(3)	0.0412(2)	0.028(1)
Cl(10)	0.2991(1)	0.7937(1)	0.1195(1)	0.040(1)
Cl(11)	0.4285(1)	0.9076(1)	0.0360(1)	0.038(1)
Cl(12)	0.2499(1)	0.9708(1)	0.0601(1)	0.039(1)
C(20)	0.2218(3)	0.0712(3)	-0.1455(2)	0.029(1)
Cl(20)	0.3387(1)	0.1107(1)	-0.1077(1)	0.036(1)
Cl(21)	0.1431(1)	0.1219(1)	-0.0904(1)	0.043(1)
Cl(22)	0.1985(1)	0.0974(1)	-0.2513(1)	0.064(1)
C(30)	-0.1243(3)	0.1955(3)	0.3557(3)	0.040(1)
Cl(30)	-0.0508(4)	0.2980(3)	0.3759(6)	0.171(4)
Cl(31)	-0.2045(2)	0.1985(4)	0.4234(2)	0.092(2)
Cl(32)	-0.0559(2)	0.1071(2)	0.3680(3)	0.078(2)
Cl(33)	-0.0266(5)	0.2459(11)	0.3281(4)	0.154(7)
Cl(34)	-0.0963(10)	0.1036(5)	0.4226(6)	0.144(6)
Cl(35)	-0.1721(10)	0.2810(11)	0.3974(8)	0.145(9)
C(40)	0.0608(3)	-0.0985(3)	0.2952(3)	0.039(1)
Cl(40)	0.1318(1)	-0.1324(1)	0.2236(1)	0.060(1)
Cl(41)	0.0219(1)	-0.1945(1)	0.3484(1)	0.076(1)
Cl(42)	0.1229(1)	-0.0168(1)	0.3652(1)	0.080(1)
C(50)	0.1891(4)	0.4095(4)	-0.4208(4)	0.054(1)
Cl(50)	0.1901(1)	0.3482(1)	-0.3292(1)	0.077(1)
Cl(51)	0.2306(3)	0.5213(2)	-0.3987(2)	0.161(2)
Cl(52)	0.0747(2)	0.3918(3)	-0.4747(2)	0.129(1)
C(60)	0.1863(3)	0.6082(3)	-0.0936(3)	0.039(1)
Cl(60)	0.3012(1)	0.6079(1)	-0.0385(1)	0.041(1)
Cl(61)	0.1782(1)	0.5412(2)	-0.1842(1)	0.082(1)

Cl(62)	0.1038(1)	0.5643(1)	-0.0319(1)	0.061(1)
C(70)	-0.0123(3)	1.1739(4)	0.1090(4)	0.048(1)
Cl(70)	0.0516(1)	1.0769(1)	0.1273(1)	0.069(1)
Cl(71)	0.0482(1)	1.2710(1)	0.1614(2)	0.091(1)
Cl(72)	-0.0359(1)	1.1933(1)	0.0026(1)	0.078(1)

Table 7. Bond lengths [Å] and angles [°] for complex *trans*-2c $[(C_5H_{10}N_2)Pd(PPh_3)_2Cl]^+ Cl^- \cdot 7\ CHCl_3$.

Pd(1)-C(1)	1.975(3)	Pd(1)-P(1)	2.3390(8)
Pd(1)-P(2)	2.3474(8)	Pd(1)-Cl(1)	2.3559(7)
P(1)-C(11)	1.818(3)	P(1)-C(31)	1.818(3)
P(1)-C(21)	1.814(3)	P(2)-C(51)	1.815(3)
P(2)-C(61)	1.825(3)	P(2)-C(41)	1.829(3)
N(1)-C(1)	1.323(4)	N(1)-C(5)	1.455(4)
N(1)-C(2)	1.475(4)	N(2)-C(1)	1.329(4)
N(2)-C(4)	1.440(4)	N(2)-C(3)	1.468(4)
C(2)-C(3)	1.532(5)	C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900	C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900	C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800	C(4)-H(4C)	0.9800
C(5)-H(5A)	0.9800	C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800	C(11)-C(12)	1.399(5)
C(11)-C(16)	1.399(5)	C(12)-C(13)	1.395(5)
C(12)-H(12)	0.9500	C(13)-C(14)	1.388(6)
C(13)-H(13)	0.9500	C(14)-C(15)	1.382(6)
C(14)-H(14)	0.9500	C(15)-C(16)	1.393(5)
C(15)-H(15)	0.9500	C(16)-H(16)	0.9500
C(21)-C(22)	1.399(5)	C(21)-C(26)	1.398(5)
C(22)-C(23)	1.381(5)	C(22)-H(22)	0.9500
C(23)-C(24)	1.395(6)	C(23)-H(23)	0.9500
C(24)-C(25)	1.397(5)	C(24)-H(24)	0.9500
C(25)-C(26)	1.379(5)	C(25)-H(25)	0.9500
C(26)-H(26)	0.9500	C(31)-C(36)	1.394(5)
C(31)-C(32)	1.399(5)	C(32)-C(33)	1.381(6)
C(32)-H(32)	0.9500	C(33)-C(34)	1.392(7)

C(33)-H(33)	0.9500	C(34)-C(35)	1.375(6)
C(34)-H(34)	0.9500	C(35)-C(36)	1.383(5)
C(35)-H(35)	0.9500	C(36)-H(36)	0.9500
C(41)-C(42)	1.392(5)	C(41)-C(46)	1.400(5)
C(42)-C(43)	1.392(5)	C(42)-H(42)	0.9500
C(43)-C(44)	1.388(6)	C(43)-H(43)	0.9500
C(44)-C(45)	1.385(6)	C(44)-H(44)	0.9500
C(45)-C(46)	1.387(5)	C(45)-H(45)	0.9500
C(46)-H(46)	0.9500	C(51)-C(56)	1.398(5)
C(51)-C(52)	1.401(4)	C(52)-C(53)	1.389(5)
C(52)-H(52)	0.9500	C(53)-C(54)	1.379(5)
C(53)-H(53)	0.9500	C(54)-C(55)	1.393(5)
C(54)-H(54)	0.9500	C(55)-C(56)	1.391(5)
C(55)-H(55)	0.9500	C(56)-H(56)	0.9500
C(61)-C(62)	1.383(5)	C(61)-C(66)	1.396(5)
C(62)-C(63)	1.398(6)	C(62)-H(62)	0.9500
C(63)-C(64)	1.375(7)	C(63)-H(63)	0.9500
C(64)-C(65)	1.379(7)	C(64)-H(64)	0.9500
C(65)-C(66)	1.385(6)	C(65)-H(65)	0.9500
C(66)-H(66)	0.9500	C(10)-Cl(12)	1.758(4)
C(10)-Cl(11)	1.764(4)	C(10)-Cl(10)	1.764(4)
C(10)-H(10)	1.0000	C(20)-Cl(21)	1.753(4)
C(20)-Cl(20)	1.757(4)	C(20)-Cl(22)	1.763(4)
C(20)-H(20)	1.0000	C(30)-Cl(35)	1.662(8)
C(30)-Cl(33)	1.659(7)	C(30)-Cl(32)	1.690(6)
C(30)-Cl(31)	1.714(5)	C(30)-Cl(30)	1.761(6)
C(30)-Cl(34)	1.778(8)	C(30)-H(30)	1.0000
C(40)-Cl(42)	1.739(5)	C(40)-Cl(41)	1.755(5)
C(40)-Cl(40)	1.755(5)	C(40)-H(40)	1.0000
C(50)-Cl(51)	1.709(6)	C(50)-Cl(50)	1.750(6)
C(50)-Cl(52)	1.752(7)	C(50)-H(50)	1.0000
C(60)-Cl(61)	1.747(5)	C(60)-Cl(62)	1.754(5)
C(60)-Cl(60)	1.770(5)	C(60)-H(60)	1.0000
C(70)-Cl(71)	1.748(5)	C(70)-Cl(70)	1.763(5)
C(70)-Cl(72)	1.750(6)	C(70)-H(70)	1.0000

C(1)-Pd(1)-P(1)	88.49(9)	C(1)-Pd(1)-P(2)	88.26(9)
P(1)-Pd(1)-P(2)	176.01(3)	C(1)-Pd(1)-Cl(1)	177.27(9)
P(1)-Pd(1)-Cl(1)	89.61(3)	P(2)-Pd(1)-Cl(1)	93.73(3)
C(11)-P(1)-C(31)	103.84(15)	C(11)-P(1)-C(21)	103.20(15)
C(31)-P(1)-C(21)	108.80(15)	C(11)-P(1)-Pd(1)	115.08(10)

C(31)-P(1)-Pd(1)	109.79(11)	C(21)-P(1)-Pd(1)	115.31(11)
C(51)-P(2)-C(61)	106.09(14)	C(51)-P(2)-C(41)	104.80(14)
C(61)-P(2)-C(41)	103.03(15)	C(51)-P(2)-Pd(1)	112.27(10)
C(61)-P(2)-Pd(1)	115.32(11)	C(41)-P(2)-Pd(1)	114.28(10)
C(1)-N(1)-C(5)	126.4(3)	C(1)-N(1)-C(2)	112.4(3)
C(5)-N(1)-C(2)	121.2(3)	C(1)-N(2)-C(4)	126.8(3)
C(1)-N(2)-C(3)	112.1(3)	C(4)-N(2)-C(3)	121.1(3)
N(1)-C(1)-N(2)	110.2(3)	N(1)-C(1)-Pd(1)	124.3(2)
N(2)-C(1)-Pd(1)	125.5(2)	N(1)-C(2)-C(3)	102.2(3)
N(1)-C(2)-H(2A)	111.3	C(3)-C(2)-H(2A)	111.3
N(1)-C(2)-H(2B)	111.3	C(3)-C(2)-H(2B)	111.3
H(2A)-C(2)-H(2B)	109.2	N(2)-C(3)-C(2)	102.9(3)
N(2)-C(3)-H(3A)	111.2	C(2)-C(3)-H(3A)	111.2
N(2)-C(3)-H(3B)	111.2	C(2)-C(3)-H(3B)	111.2
H(3A)-C(3)-H(3B)	109.1	N(2)-C(4)-H(4A)	109.5
N(2)-C(4)-H(4B)	109.5	H(4A)-C(4)-H(4B)	109.5
N(2)-C(4)-H(4C)	109.5	H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5	N(1)-C(5)-H(5A)	109.5
N(1)-C(5)-H(5B)	109.5	H(5A)-C(5)-H(5B)	109.5
N(1)-C(5)-H(5C)	109.5	H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5	C(12)-C(11)-C(16)	119.1(3)
C(12)-C(11)-P(1)	121.7(3)	C(16)-C(11)-P(1)	119.1(3)
C(13)-C(12)-C(11)	119.9(4)	C(13)-C(12)-H(12)	120.1
C(11)-C(12)-H(12)	120.1	C(12)-C(13)-C(14)	120.4(4)
C(12)-C(13)-H(13)	119.8	C(14)-C(13)-H(13)	119.8
C(15)-C(14)-C(13)	120.1(3)	C(15)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9	C(14)-C(15)-C(16)	119.9(4)
C(14)-C(15)-H(15)	120.0	C(16)-C(15)-H(15)	120.0
C(15)-C(16)-C(11)	120.6(4)	C(15)-C(16)-H(16)	119.7
C(11)-C(16)-H(16)	119.7	C(22)-C(21)-C(26)	119.1(3)
C(22)-C(21)-P(1)	120.6(3)	C(26)-C(21)-P(1)	120.3(2)
C(23)-C(22)-C(21)	120.5(3)	C(23)-C(22)-H(22)	119.8
C(21)-C(22)-H(22)	119.8	C(22)-C(23)-C(24)	120.3(3)
C(22)-C(23)-H(23)	119.9	C(24)-C(23)-H(23)	119.9
C(23)-C(24)-C(25)	119.3(3)	C(23)-C(24)-H(24)	120.4
C(25)-C(24)-H(24)	120.4	C(26)-C(25)-C(24)	120.5(3)
C(26)-C(25)-H(25)	119.7	C(24)-C(25)-H(25)	119.7
C(25)-C(26)-C(21)	120.3(3)	C(25)-C(26)-H(26)	119.8
C(21)-C(26)-H(26)	119.8	C(36)-C(31)-C(32)	119.0(3)
C(36)-C(31)-P(1)	119.5(3)	C(32)-C(31)-P(1)	121.4(3)
C(33)-C(32)-C(31)	119.4(4)	C(33)-C(32)-H(32)	120.3

C(31)-C(32)-H(32)	120.3	C(32)-C(33)-C(34)	120.9(4)
C(32)-C(33)-H(33)	119.6	C(34)-C(33)-H(33)	119.6
C(35)-C(34)-C(33)	120.0(4)	C(35)-C(34)-H(34)	120.0
C(33)-C(34)-H(34)	120.0	C(36)-C(35)-C(34)	119.6(4)
C(36)-C(35)-H(35)	120.2	C(34)-C(35)-H(35)	120.2
C(35)-C(36)-C(31)	121.1(3)	C(35)-C(36)-H(36)	119.5
C(31)-C(36)-H(36)	119.5	C(42)-C(41)-C(46)	118.8(3)
C(42)-C(41)-P(2)	121.0(3)	C(46)-C(41)-P(2)	120.0(3)
C(41)-C(42)-C(43)	120.2(4)	C(41)-C(42)-H(42)	119.9
C(43)-C(42)-H(42)	119.9	C(44)-C(43)-C(42)	120.5(4)
C(44)-C(43)-H(43)	119.7	C(42)-C(43)-H(43)	119.7
C(45)-C(44)-C(43)	119.5(3)	C(45)-C(44)-H(44)	120.3
C(43)-C(44)-H(44)	120.3	C(44)-C(45)-C(46)	120.3(4)
C(44)-C(45)-H(45)	119.9	C(46)-C(45)-H(45)	119.9
C(45)-C(46)-C(41)	120.6(4)	C(45)-C(46)-H(46)	119.7
C(41)-C(46)-H(46)	119.7	C(56)-C(51)-C(52)	119.1(3)
C(56)-C(51)-P(2)	119.3(2)	C(52)-C(51)-P(2)	121.5(2)
C(53)-C(52)-C(51)	120.2(3)	C(53)-C(52)-H(52)	119.9
C(51)-C(52)-H(52)	119.9	C(54)-C(53)-C(52)	120.3(3)
C(54)-C(53)-H(53)	119.9	C(52)-C(53)-H(53)	119.9
C(53)-C(54)-C(55)	120.2(3)	C(53)-C(54)-H(54)	119.9
C(55)-C(54)-H(54)	119.9	C(56)-C(55)-C(54)	119.9(3)
C(56)-C(55)-H(55)	120.0	C(54)-C(55)-H(55)	120.0
C(55)-C(56)-C(51)	120.2(3)	C(55)-C(56)-H(56)	119.9
C(51)-C(56)-H(56)	119.9	C(62)-C(61)-C(66)	119.0(3)
C(62)-C(61)-P(2)	121.4(3)	C(66)-C(61)-P(2)	119.6(3)
C(61)-C(62)-C(63)	120.0(4)	C(61)-C(62)-H(62)	120.0
C(63)-C(62)-H(62)	120.0	C(64)-C(63)-C(62)	120.6(4)
C(64)-C(63)-H(63)	119.7	C(62)-C(63)-H(63)	119.7
C(63)-C(64)-C(65)	119.5(4)	C(63)-C(64)-H(64)	120.3
C(65)-C(64)-H(64)	120.3	C(64)-C(65)-C(66)	120.5(4)
C(64)-C(65)-H(65)	119.8	C(66)-C(65)-H(65)	119.8
C(65)-C(66)-C(61)	120.4(4)	C(65)-C(66)-H(66)	119.8
C(61)-C(66)-H(66)	119.8	Cl(12)-C(10)-Cl(11)	110.4(2)
Cl(12)-C(10)-Cl(10)	110.1(2)	Cl(11)-C(10)-Cl(10)	110.4(2)
Cl(12)-C(10)-H(10)	108.6	Cl(11)-C(10)-H(10)	108.6
Cl(10)-C(10)-H(10)	108.6	Cl(21)-C(20)-Cl(20)	111.3(2)
Cl(21)-C(20)-Cl(22)	109.9(2)	Cl(20)-C(20)-Cl(22)	108.6(2)
Cl(21)-C(20)-H(20)	109.0	Cl(20)-C(20)-H(20)	109.0
Cl(22)-C(20)-H(20)	109.0	Cl(35)-C(30)-Cl(33)	103.5(10)
Cl(35)-C(30)-Cl(32)	149.2(5)	Cl(33)-C(30)-Cl(32)	80.6(6)

Cl(35)-C(30)-Cl(31)	47.2(7)	Cl(33)-C(30)-Cl(31)	145.4(6)
Cl(32)-C(30)-Cl(31)	114.8(4)	Cl(35)-C(30)-Cl(30)	64.6(7)
Cl(33)-C(30)-Cl(30)	40.7(5)	Cl(32)-C(30)-Cl(30)	107.9(4)
Cl(31)-C(30)-Cl(30)	105.2(4)	Cl(35)-C(30)-Cl(34)	115.6(8)
Cl(33)-C(30)-Cl(34)	109.6(7)	Cl(32)-C(30)-Cl(34)	38.0(5)
Cl(31)-C(30)-Cl(34)	77.1(6)	Cl(30)-C(30)-Cl(34)	115.8(5)
Cl(35)-C(30)-H(30)	100.8	Cl(33)-C(30)-H(30)	91.9
Cl(32)-C(30)-H(30)	109.6	Cl(31)-C(30)-H(30)	109.6
Cl(30)-C(30)-H(30)	109.6	Cl(34)-C(30)-H(30)	130.4
Cl(42)-C(40)-Cl(41)	110.0(3)	Cl(42)-C(40)-Cl(40)	110.4(3)
Cl(41)-C(40)-Cl(40)	109.6(3)	Cl(42)-C(40)-H(40)	108.9
Cl(41)-C(40)-H(40)	108.9	Cl(40)-C(40)-H(40)	108.9
Cl(51)-C(50)-Cl(50)	110.2(3)	Cl(51)-C(50)-Cl(52)	115.9(4)
Cl(50)-C(50)-Cl(52)	106.6(3)	Cl(51)-C(50)-H(50)	107.9
Cl(50)-C(50)-H(50)	107.9	Cl(52)-C(50)-H(50)	107.9
Cl(61)-C(60)-Cl(62)	110.2(3)	Cl(61)-C(60)-Cl(60)	108.8(3)
Cl(62)-C(60)-Cl(60)	109.9(2)	Cl(61)-C(60)-H(60)	109.3
Cl(62)-C(60)-H(60)	109.3	Cl(60)-C(60)-H(60)	109.3
Cl(71)-C(70)-Cl(70)	111.0(3)	Cl(71)-C(70)-Cl(72)	110.4(3)
Cl(70)-C(70)-Cl(72)	110.5(3)	Cl(71)-C(70)-H(70)	108.3
Cl(70)-C(70)-H(70)	108.3	Cl(72)-C(70)-H(70)	108.3

Table 8. Anisotropic displacement parameters (Å²) for complex *trans*-2c $[(C_5H_{10}N_2)Pd(PPh_3)_2Cl]^+ Cl^- \cdot 7\ CHCl_3$.

The anisotropic displacement factor exponent takes the form:
$-2\pi^2[\ h^2 a^{*2} U_{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd(1)	0.020(1)	0.013(1)	0.014(1)	0.000(1)	0.003(1)	0.003(1)
Cl(1)	0.031(1)	0.018(1)	0.017(1)	-0.001(1)	0.006(1)	0.006(1)
Cl(2)	0.022(1)	0.030(1)	0.025(1)	-0.003(1)	0.004(1)	0.003(1)
P(1)	0.023(1)	0.013(1)	0.016(1)	0.000(1)	0.003(1)	0.003(1)
P(2)	0.022(1)	0.015(1)	0.015(1)	0.001(1)	0.004(1)	0.003(1)
N(1)	0.021(1)	0.022(1)	0.022(1)	-0.003(1)	0.006(1)	0.002(1)
N(2)	0.022(1)	0.018(1)	0.019(1)	-0.003(1)	0.003(1)	0.003(1)

C(1)	0.020(1)	0.015(1)	0.017(1)	0.000(1)	0.002(1)	0.004(1)
C(2)	0.024(2)	0.028(2)	0.024(2)	-0.002(1)	0.009(1)	0.009(1)
C(3)	0.029(2)	0.024(2)	0.020(1)	-0.007(1)	0.006(1)	0.004(1)
C(4)	0.021(1)	0.023(2)	0.026(2)	-0.003(1)	0.002(1)	0.001(1)
C(5)	0.022(2)	0.030(2)	0.031(2)	-0.002(1)	0.005(1)	-0.002(1)
C(11)	0.029(2)	0.017(1)	0.017(1)	0.000(1)	0.002(1)	0.006(1)
C(12)	0.034(2)	0.019(1)	0.021(1)	-0.001(1)	0.002(1)	0.001(1)
C(13)	0.049(2)	0.020(2)	0.024(2)	-0.003(1)	0.004(2)	0.000(1)
C(14)	0.059(3)	0.022(2)	0.021(2)	0.002(1)	0.007(2)	0.014(2)
C(15)	0.043(2)	0.030(2)	0.023(2)	0.002(1)	0.009(2)	0.016(2)
C(16)	0.031(2)	0.022(2)	0.025(2)	0.001(1)	0.007(1)	0.007(1)
C(21)	0.025(2)	0.019(1)	0.017(1)	0.001(1)	0.001(1)	0.003(1)
C(22)	0.033(2)	0.019(1)	0.029(2)	0.005(1)	-0.003(1)	0.002(1)
C(23)	0.036(2)	0.030(2)	0.032(2)	0.006(1)	-0.004(2)	0.009(2)
C(24)	0.032(2)	0.033(2)	0.030(2)	-0.003(1)	-0.008(2)	0.005(2)
C(25)	0.031(2)	0.025(2)	0.028(2)	-0.005(1)	-0.003(1)	0.004(1)
C(26)	0.029(2)	0.018(1)	0.025(2)	-0.002(1)	0.003(1)	0.006(1)
C(31)	0.027(2)	0.019(1)	0.017(1)	-0.002(1)	0.005(1)	0.000(1)
C(32)	0.031(2)	0.040(2)	0.025(2)	0.013(2)	0.007(1)	0.007(2)
C(33)	0.041(2)	0.062(3)	0.033(2)	0.024(2)	0.012(2)	0.005(2)
C(34)	0.034(2)	0.057(3)	0.033(2)	0.009(2)	0.012(2)	-0.004(2)
C(35)	0.030(2)	0.038(2)	0.034(2)	0.003(2)	0.007(2)	0.002(2)
C(36)	0.028(2)	0.022(2)	0.028(2)	0.002(1)	0.002(1)	0.002(1)
C(41)	0.029(2)	0.016(1)	0.015(1)	0.001(1)	0.004(1)	0.002(1)
C(42)	0.034(2)	0.021(1)	0.020(1)	0.002(1)	0.008(1)	0.004(1)
C(43)	0.048(2)	0.026(2)	0.020(2)	0.001(1)	0.011(2)	0.009(2)
C(44)	0.055(2)	0.027(2)	0.017(1)	-0.001(1)	0.004(2)	0.010(2)
C(45)	0.044(2)	0.030(2)	0.024(2)	-0.005(1)	-0.004(2)	0.002(2)
C(46)	0.032(2)	0.025(2)	0.022(2)	-0.001(1)	0.003(1)	0.001(1)
C(51)	0.022(1)	0.014(1)	0.020(1)	0.002(1)	0.004(1)	0.003(1)
C(52)	0.027(2)	0.019(1)	0.020(1)	0.003(1)	0.003(1)	0.003(1)
C(53)	0.033(2)	0.020(1)	0.025(2)	0.005(1)	0.005(1)	0.000(1)
C(54)	0.030(2)	0.021(2)	0.030(2)	0.002(1)	0.004(1)	-0.004(1)
C(55)	0.031(2)	0.024(2)	0.023(2)	0.000(1)	0.002(1)	-0.004(1)
C(56)	0.027(2)	0.021(1)	0.019(1)	0.002(1)	0.003(1)	0.000(1)
C(61)	0.023(1)	0.019(1)	0.020(1)	-0.001(1)	0.002(1)	0.002(1)
C(62)	0.024(2)	0.039(2)	0.036(2)	0.015(2)	0.007(2)	0.004(1)
C(63)	0.024(2)	0.062(3)	0.049(3)	0.018(2)	0.013(2)	0.004(2)
C(64)	0.024(2)	0.041(2)	0.048(2)	-0.005(2)	0.004(2)	0.008(2)
C(65)	0.032(2)	0.032(2)	0.056(3)	0.008(2)	0.004(2)	0.013(2)
C(66)	0.031(2)	0.028(2)	0.049(2)	0.015(2)	0.013(2)	0.011(1)

C(10)	0.027(2)	0.030(2)	0.027(2)	-0.004(1)	0.003(1)	0.005(1)
Cl(10)	0.051(1)	0.027(1)	0.042(1)	0.005(1)	0.007(1)	0.010(1)
Cl(11)	0.030(1)	0.052(1)	0.034(1)	-0.007(1)	0.005(1)	0.006(1)
Cl(12)	0.042(1)	0.030(1)	0.049(1)	0.009(1)	0.017(1)	0.014(1)
C(20)	0.026(2)	0.033(2)	0.028(2)	-0.004(1)	0.004(1)	0.005(1)
Cl(20)	0.029(1)	0.046(1)	0.032(1)	-0.002(1)	0.005(1)	-0.004(1)
Cl(21)	0.040(1)	0.048(1)	0.048(1)	0.004(1)	0.021(1)	0.015(1)
Cl(22)	0.048(1)	0.118(1)	0.027(1)	0.002(1)	-0.002(1)	0.025(1)
C(30)	0.037(2)	0.055(3)	0.029(2)	0.000(2)	0.005(2)	0.007(2)
Cl(30)	0.175(6)	0.057(2)	0.302(10)	-0.028(3)	0.135(6)	-0.038(2)
Cl(31)	0.046(1)	0.181(5)	0.058(1)	0.006(2)	0.024(1)	0.027(2)
Cl(32)	0.057(2)	0.070(2)	0.104(3)	-0.026(2)	-0.012(2)	0.028(1)
Cl(33)	0.078(5)	0.290(16)	0.067(4)	0.082(6)	-0.022(3)	-0.093(7)
Cl(34)	0.241(13)	0.069(4)	0.089(6)	0.034(4)	-0.055(7)	-0.040(5)
Cl(35)	0.165(12)	0.154(13)	0.104(8)	-0.081(9)	-0.067(8)	0.112(10)
C(40)	0.030(2)	0.047(2)	0.042(2)	-0.006(2)	0.004(2)	0.010(2)
Cl(40)	0.066(1)	0.073(1)	0.048(1)	-0.003(1)	0.018(1)	0.023(1)
Cl(41)	0.057(1)	0.088(1)	0.089(1)	0.028(1)	0.025(1)	0.012(1)
Cl(42)	0.064(1)	0.079(1)	0.092(1)	-0.043(1)	-0.008(1)	0.019(1)
C(50)	0.057(3)	0.053(3)	0.056(3)	-0.009(2)	0.024(3)	0.005(2)
Cl(50)	0.066(1)	0.089(1)	0.085(1)	0.021(1)	0.029(1)	0.018(1)
Cl(51)	0.303(4)	0.068(1)	0.131(2)	-0.044(1)	0.144(3)	-0.064(2)
Cl(52)	0.093(2)	0.207(3)	0.093(2)	0.050(2)	0.011(1)	0.044(2)
C(60)	0.041(2)	0.040(2)	0.037(2)	0.010(2)	0.007(2)	0.001(2)
Cl(60)	0.047(1)	0.040(1)	0.034(1)	0.007(1)	0.000(1)	-0.002(1)
Cl(61)	0.067(1)	0.126(2)	0.044(1)	-0.030(1)	0.012(1)	-0.049(1)
Cl(62)	0.056(1)	0.066(1)	0.074(1)	0.027(1)	0.037(1)	0.021(1)
C(70)	0.026(2)	0.046(3)	0.075(4)	-0.009(2)	0.016(2)	0.001(2)
Cl(70)	0.044(1)	0.046(1)	0.121(2)	0.009(1)	0.029(1)	0.006(1)
Cl(71)	0.043(1)	0.066(1)	0.154(2)	-0.041(1)	-0.016(1)	0.012(1)
Cl(72)	0.074(1)	0.094(1)	0.074(1)	-0.005(1)	0.026(1)	0.034(1)